

Argonne National Laboratory

THE CRYSTAL STRUCTURE OF DISODIUM
TETRANITRITONITROSOHYDROXYRUTHENATE(III)
2-HYDRATE BY NEUTRON DIFFRACTION

by

M. H. Mueller and S. H. Simonsen

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DETERMINATION OF CRYSTAL STRUCTURE
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Metallurgy Division

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ABSTRACT

The crystal structure of $\text{Na}_2[\text{Ru}(\text{NO}_2)_4(\text{NO})(\text{OH})] \cdot 2\text{H}_2\text{O}$ was investigated by neutron diffraction, and the positional parameters of the heavy and light atoms were determined. The unit cell is monoclinic: $a_0 = 12.75$; $b_0 = 14.52$; $c_0 = 7.37\text{\AA}$; $\beta = 121.20^\circ$. The space group is $C2/m$, with 4 molecules (100 atoms) per unit cell and systematic absences are $h+k = 2n+1$. The structure can be considered as consisting mainly of 6-fold coordination about three central atoms, namely, Ru, Na_1 , and Na_2 , forming three different kinds of octahedra. These octahedra form an interlocking chain throughout the structure, in which common atoms or common edges are shared between the octahedra. The 6-fold coordination about the ruthenium consists of four nitrogens of the nitrito groups arranged in a square, the nitrogen of the nitroso, and the oxygen of the hydroxyl group. These ruthenium octahedra are held together by Na-O bridges involving 6-fold coordination about the two crystallographically different sodium atoms. Hydrogen bonding apparently is not important in this crystal.

INTRODUCTION

The general features of the stereochemistry of the coordination complexes of ruthenium have been established by the structure determinations of several compounds: (a) $\text{K}_4\text{Ru}_2\text{Cl}_{10}\text{O}$; (1) (b) K_2RuCl_6 ; (2) (c) $[\text{Ru}(\text{NH}_3)_4(\text{NO})(\text{OH})]\text{Cl}_2$; (3) (d) $(\text{NH}_4)_2[\text{RuCl}_4(\text{NO})(\text{OH})]$; (4) and (e) $\text{K}_2[\text{Ru}(\text{NO}_2)_4(\text{NO})(\text{OH})]$. (5)

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However, there were some details in the structure of (c) and (d), especially the Ru-N-O bonding, that made it desirable to examine a similar type of compound, particularly in view of the current interest in ruthenium nitrosyl complexes. Also, all the previous structures had been solved by projections and the more accurate bond lengths attainable from three-dimensional data were desired. The structure of $\text{Na}_2[\text{Ru}(\text{NO}_2)_4(\text{NO})(\text{OH})] \cdot 2\text{H}_2\text{O}$ was determined by neutron diffraction for several reasons:

(1) We wished to demonstrate the power of the neutron diffraction method in the complete solution of a fairly complex structure, applying the standard techniques used in X-ray determinations. No X-ray work had been done on the compound and its structure was unknown at the start of the investigation. At a later point in the work, some X-ray zone intensity data were collected to illustrate the difference in the X-ray and neutron Fouriers.

(2) Because ruthenium contributes so greatly to the scattering in the case of X rays, the accuracy of the light-atom parameters is affected. In the case of neutrons, the scattering contribution by all atoms is more nearly equal, so that all atoms are located with about equal precision.

(3) Information concerning the role of possible hydrogen bonding required knowledge of the hydrogen positions, attainable best by neutron diffraction.

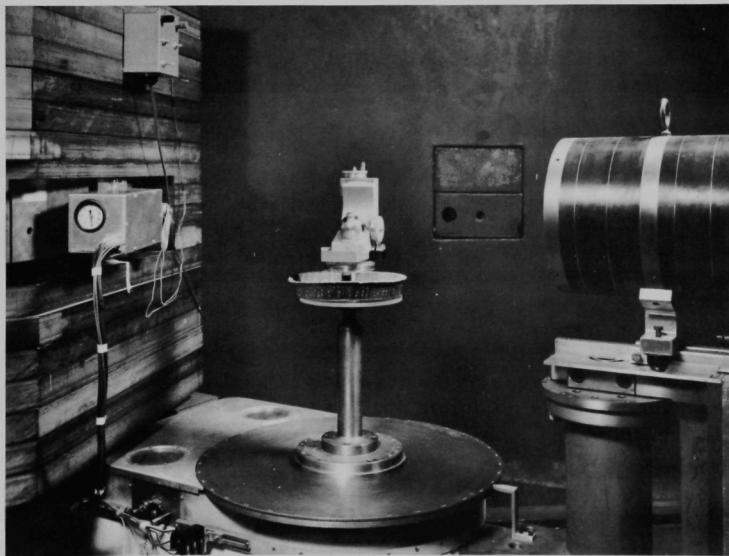
The preliminary results of this investigation have been reported in the Metallurgy Division Annual Reports listed on the title page. A summary was also presented orally at the International Union of Crystallography Sixth International Congress held in Rome, Italy, September 9-18, 1963 and was published in their Abstracts.⁽⁶⁾ A paper⁽⁷⁾ has also been prepared and submitted for publication. However, since it was not possible or planned to include in the above publications many of the important details of the experimental technique or the listing of the final agreement between the observed and calculated structure factors of approximately 2000 reflections, this report has been prepared.

EXPERIMENTAL

Pollack and Wallace⁽⁸⁾ prepared large crystals in the following way: Sodium nitrite, slightly in excess of the stoichiometric amount, was added to an aqueous solution of ruthenium(IV) chloride. The solution was heated until a red color developed and was then allowed to cool slowly. The crystals were large, well-formed, reddish-orange prisms.

The unit-cell dimensions were obtained conventionally from rotation, Weissenberg, and precession X-ray photographs. The cell was monoclinic, with the following dimensions: $a = 12.75$; $b = 14.52$; $c = 7.37 \text{ \AA}$; $\beta = 121.20^\circ$. The systematic absences ($h+k = 2n+1$) indicated the possible space groups C2, Cm, or C2/m. The density, measured by displacement of carbon tetrachloride, was found to be 2.29 g cm^{-3} . The calculated density with $z = 4$, is 2.36 g cm^{-3} .

A single crystal, in the form of a cube 0.46 cm on an edge, was positioned on a GE Single Crystal Orienter mounted on Neutron Spectrometer II at the Argonne CP-5 reactor, as shown in Figure 1. A neutron wavelength of 1.16 \AA , reflected from the (111) face of a copper single crystal, was used. The neutron flux at the sample was approximately $10^6 \text{ neutrons cm}^{-2} \text{ sec}^{-1}$.



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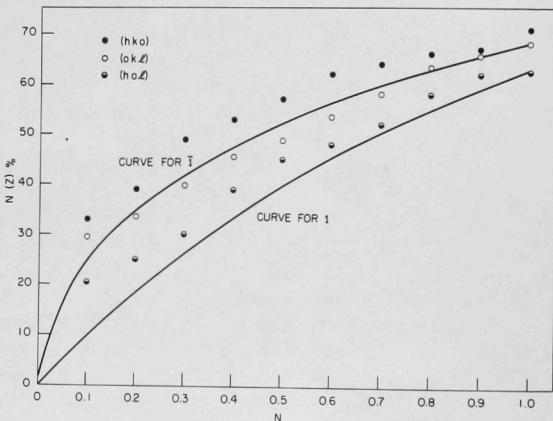
Fig. 1. Photo of Single Crystal Orienter as Positioned on the Argonne Neutron Spectrometer II

Integrated intensities were obtained by a θ - 2θ scan after phi and chi angles on the orienter had been set manually. The primary beam was monitored with a fission counter acting as the timing device for the counting intervals. The scaler count and angle were printed out on a typewriter at each interval of $0.10^\circ 2\theta$ and the scaler reset. Integrated intensity = (Σ interval counts) - (number of intervals x average background per interval). These integrated intensities were multiplied by the Lorentz correction ($\sin 2\theta$) to obtain F^2 values. No correction was made for absorption because the transmission was high (approximately 80%) and the sample was symmetrically shaped. A more detailed description of this instrument and the techniques used is given in an ANL report.⁽⁹⁾

Integrated intensities of 1359 reflections were measured: 567 more were below the limit of measurement. Another 301 reflections were available in the sphere of reflection, but unfortunately the crystal was destroyed accidentally before measurements were completed.

DETERMINATION OF STRUCTURE

The statistical test of Howells *et al.*⁽¹⁰⁾ was applied to the intensities of the $(hk0)$, $(0k\ell)$, and $(0kl)$ zones, the range $\sin \theta = 0-0.2$ being disregarded. The results, shown in Figure 2, indicate the space group to be $C2/m$, also suggested by the morphology of the crystal.



106-5674

Fig. 2. Distribution for Intensities of $(0kl)$, $(0k\ell)$, and $(hk0)$ Zones of Disodium Tetranitrito-nitrosohydroxyruthenate(III) 2-Hydrate Compared with Theoretical Curves for I and \bar{I}

Howells, Phillips, and Rogers⁽¹⁰⁾ derived distribution functions of intensities for noncentrosymmetric and centrosymmetric crystals, and showed that the percentage, $N(z)\%$, of the reflections whose intensities are less than or equal to $z (= I/\langle I \rangle)$, a fraction of the local average intensity, is given by:

$$N(z)\% = 1 - \exp(-z) \cdot 100 \text{ for a noncentrosymmetric crystal, and}$$

$$N(z)\% = \operatorname{erf}(z/2)^{1/2} \cdot 100 \text{ (where } \operatorname{erf} \text{ is the error function) for a centrosymmetric crystal.}$$

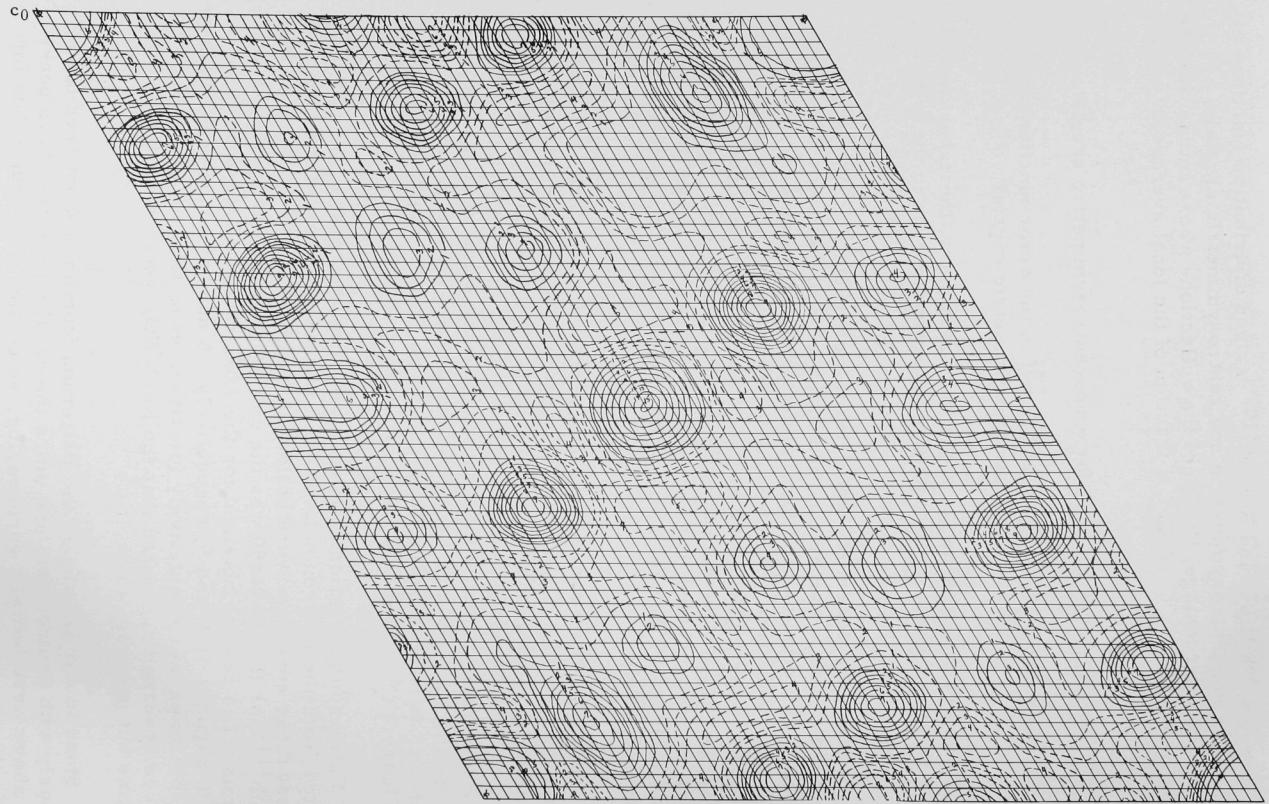
To detect the presence of a center of symmetry, the experimental data are compared graphically with the theoretical curves in the following way.

Because the observed intensities fall off rapidly in $\langle I \rangle$ with increasing $\sin \theta$ due to thermal motion in the case of neutron scattering, and to thermal motion and the form factors in the case of X-ray scattering, only the intensities within a small range of $\sin \theta$ are compared. The reflections and their intensities are arranged in order of increasing $\sin \theta$, weighting each reflection with the appropriate multiplicity. Systematic absences are not included, but accidental absences are given intensities of zero and included in the tabulation. Reflections having $\sin \theta$ less than 0.200 are not used.

The reflections are divided into several groups, each group containing about an equal number of reflections, and the average intensity $\langle I \rangle$ determined for each group. The value of $N(z)$ for $z = 0.1$ is obtained by counting the number of reflections having intensities less than or equal to $0.1 \langle I \rangle$ and dividing by the total number of reflections in the group. Values $N(0.2), N(0.3), \dots, N(1.0)$ are found in a similar way. Each group is treated separately; the corresponding $N(z)$ values are then averaged for plotting, as in Figure 2 (N in Figure 2 corresponds to z).

Patterson projections, showing well-resolved peaks, were first computed from the neutron data of the three axial zones. At the time in 1960 that these zone data were collected the Pittsburgher 2-dimensional program⁽¹¹⁾ for the IBM-650 was the only working Fourier program available to us. The results obtained for the $h0\ell$, $hk0$, and $0k\ell$ zones are shown in Figures 3, 4, and 5, respectively. A number of the peaks in these Patterson maps were tentatively identified, especially in $h0\ell$ projection. Distances observed suggested that the Ru-N(NO₂) vectors were not in the $h0\ell$ plane but probably 45° to it.

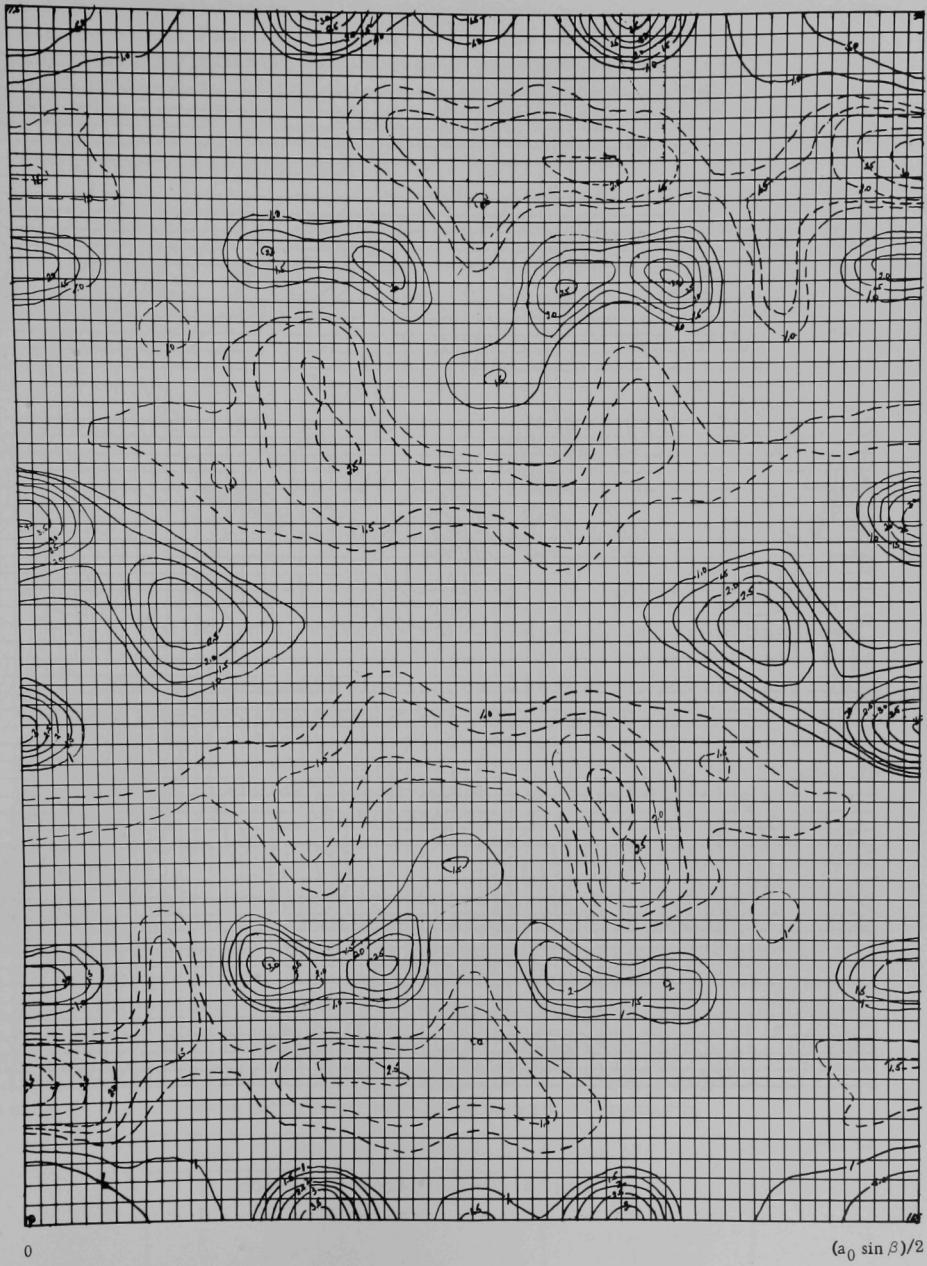
Since to our knowledge the Patterson function had not been used previously with neutron data and since the results from the sharp peaks shown above were initially encouraging, we continued to gather data for



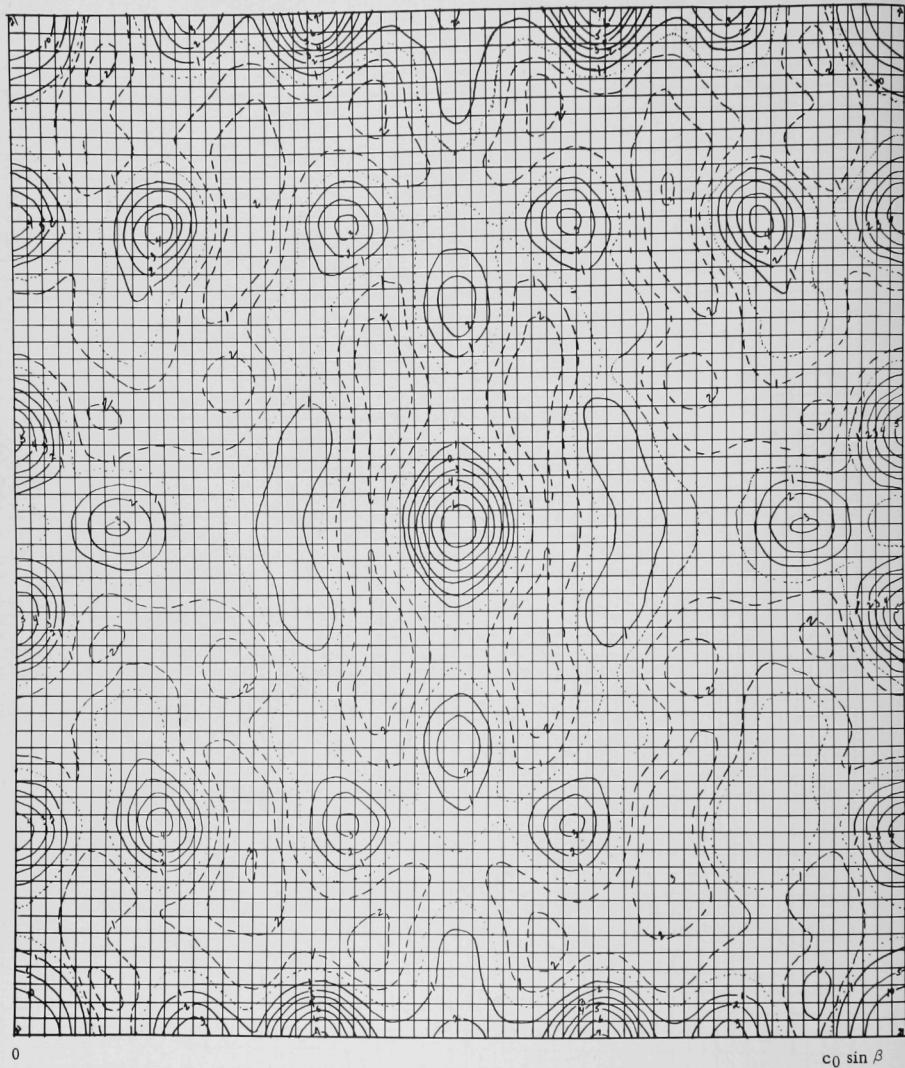
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Fig. 3. $h0\ell$ Neutron Patterson

b/2



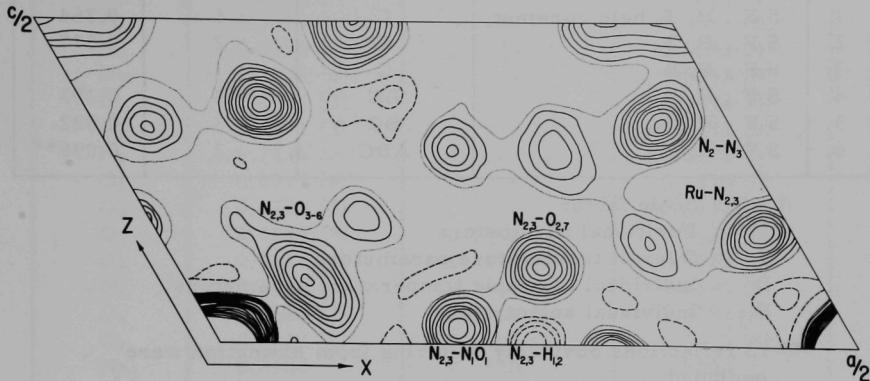
38595

$b/2$ 

38596

Fig. 5. $0kl$ Neutron Patterson

a 3-dimensional Patterson. In the meantime, we obtained the Sly-Shoemaker 3-dimensional Fourier Program⁽¹²⁾ for use with the IBM-704 computer. As a check on its successful operation we again ran the $h0\ell$ 2-dimensional data. The results replotted from the computer output together with some of the vector identities as finally determined are shown in Figure 6. Some of the shorter vectors, such as the Ru-N, N-N, and the short N-O, gave the initial hints of the structure.



38521

Fig. 6. $h0\ell$ Neutron Patterson Showing Some of the Vector Distances

The 3-dimensional Patterson, calculated by means of above MIFRI computer program, also suggested the space group to be $C2/m$, and subsequent refinements were based upon this choice. The nitrito nitrogen vectors (N_2-N_3 vectors) were readily identified in this 3-dimensional map and used as image points for a superposition map based on the Buerger minimum function.⁽¹³⁾ This was carried out on the IBM-704 by using the Penfold program.⁽¹⁴⁾

The trial structure thus obtained was refined by successive " F_0 " and " F_c " synthesis until all atoms had been located. At this point refinement was continued by use of the Busing-Levy least-squares program.⁽¹⁵⁾ To conserve computer time the reflections were divided into four groups according to Table I, and the refinement was carried out in progressive stages, as outlined in Table II.

Table I
DISTRIBUTION OF REFLECTIONS FOR REFINEMENT

Group	Number of Reflections	$\sin \theta / \lambda$ Range
A	374	0-0.1990
B	585	0.1993-0.3764
C	400	0.3765-0.5827
D	567	Unobserved

Table II
SEQUENCE OF THE LEAST-SQUARES REFINEMENT

	Parameters Refined*	Reflections Used	Number of Cycles	Final R
1.	S.F., P, T_0 held constant	C	6	0.364
2.	S.F., P, T_0	C	2	0.377
3.	S.F., P, B	C	1	
4.	S.F., P, B	BC	3	0.193
5.	S.F., P, B_{ij}	BC	3	0.082
6.	S.F., P, B_{ij}	ABC	2	0.098**

* S.F.: Scale factor

P : Positional parameters

T_0 : Overall temperature parameters

B : Individual isotropic temperature parameters

B_{ij} : Individual anisotropic

** 12 reflections obviously suffering from extinction were excluded.

The final calculation of the structure factor, based on individual anisotropic temperature parameters, gave an agreement index, $R = \Sigma(|F_0| - |F_c|)/\sum|F_0|$, of 9.8% for the observed reflections, excluding the following 12 strong, low-angle reflections: (020), (040), (080), (200), (240), (20 $\bar{2}$), (24 $\bar{2}$), (40 $\bar{2}$), (203), (10,0,3), (605), and (404). It can be noted in Table V that these reflections do show low observed F's relative to the calculated. The slightly lower R of 8.2% shown in Table II for the BC reflections is probably due to the fact that the A reflections, which have the lower value of $\sin \theta/\lambda$, generally do suffer from some extinction, and hence their inclusion increases the R to the 9.8%. When all of the unobserved reflections were included in the calculation, $R = 17.7\%$ was obtained. Some of this increase is probably due to errors in angle settings of the unobserved reflection ions.

The final least-squares positional parameters from the ABC set are given in Table III, and the anisotropic temperature parameters are shown in Table IV. A list of observed and calculated structure factors obtained from the final cycle based on the ABC set of reflections are shown in Table V. It should be noted that an asterisk in front of certain reflections in this table indicates that intensity measurements were not obtained since they were the missing reflections referred to previously.

Table III

FINAL COORDINATES AND ERRORS* OF ALL ATOMS
FROM LEAST-SQUARES RESULTS

Atom	X	Y	Z
H ₁	0.0449 (8)	0	0.8606 (15)
H ₂	0.0086 (21)	0.2080 (16)	0.1811 (22)
H ₃	0.4631 (15)	0.2190 (8)	0.2675 (29)
Ru	0.2623 (3)	0	0.0035 (5)
N ₁	0.4197 (3)	0	0.1892 (4)
N ₂	0.2311 (2)	0.1002 (1)	0.1715 (3)
N ₃	0.2835 (2)	0.1024 (1)	0.8276 (3)
O ₁	0.0875 (4)	0	0.7910 (6)
O ₂	0.4788 (5)	0	0.6911 (11)
O ₃	0.1289 (5)	0.1093 (5)	0.1420 (9)
O ₄	0.3147 (5)	0.1474 (4)	0.3021 (8)
O ₅	0.2122 (4)	0.1118 (4)	0.6391 (6)
O ₆	0.3686 (7)	0.1552 (6)	0.9151 (9)
O ₇	0.0121 (5)	0.2304 (3)	0.3021 (8)
Na ₁	0.2500	0.2500	0.5000
Na ₂	0	0.1098 (6)	0.5000

*Standard errors ($\times 10^4$) appear in parentheses.

Table IV

FINAL THERMAL PARAMETERS B_{ij}

Atom	B ₁₁	B ₂₂	B ₃₃	B ₁₂	B ₁₃	B ₂₃
H ₁	0.0052	0.0109	0.0200	0	0.0070	0
H ₂	0.0322	0.0160	0.0336	0.0039	0.0223	0.0054
H ₃	0.0201	0.0046	0.0713	-0.0035	0.0162	-0.0053
Ru	0.0037	0.0021	0.0105	0	0.0034	0
N ₁	0.0041	0.0034	0.0136	0	0.0030	0
N ₂	0.0067	0.0028	0.0151	0.0004	0.0060	-0.0009
N ₃	0.0055	0.0027	0.0158	-0.0003	0.0055	0.0010
O ₁	0.0039	0.0032	0.0128	0	0.0037	0
O ₂	0.0044	0.0071	0.0246	0	0.0014	0
O ₃	0.0080	0.0080	0.0333	0.0013	0.0102	-0.0050
O ₄	0.0103	0.0048	0.0298	-0.0020	0.0108	-0.0063
O ₅	0.0077	0.0056	0.0176	-0.0006	0.0041	0.0045
O ₆	0.0167	0.0095	0.0228	-0.0092	0.0070	-0.0002
O ₇	0.0124	0.0042	0.0233	0.0019	0.0105	0.0029
Na ₁	0.0196	0.0026	0.0449	-0.0004	0.0253	-0.0001
Na ₂	0.0049	0.0029	0.0251	0	0.0024	0

Table V

TABLE OF F_{calc} AND F_{obs} FOR ALL REFLECTIONS AFTER FINAL LEAST-SQUARES CYCLE BASED ON ABC REFLECTIONS

H	K	L	OBSERVED	CALCULATED	OBS-CAL
0	2	0	4.522	6.223	-1.700
0	4	0	6.273	-7.999	1.726
0	6	0	1.890	-1.759	-.131
0	8	0	8.972	11.705	-2.732
0	10	0	6.971	7.702	-.731
0	12	0	5.144	5.092	.052
0	14	0	2.616	-2.501	-.115
0	16	0	.793	-.335	-.458
0	18	0	3.508	3.529	-.021
0	20	0	4.439	4.510	-.070
0	22	0	2.160	1.097	1.063
1	1	0	1.899	-1.969	.070
1	3	0	2.303	-2.100	-.203
1	5	0	2.760	-2.860	.100
1	7	0	4.622	-5.109	.487
1	9	0	3.036	2.800	.236
1	11	0	2.593	-2.307	-.285
1	13	0	.688	-.800	.111
1	15	0	1.888	-1.961	.073
1	17	0	.678	.722	-.044
1	19	0	.311	-.409	.098
1	21	0	.000	-.449	.449
2	0	0	6.103	-10.518	4.415
2	2	0	.831	-.250	-.581
2	4	0	6.144	8.128	-1.985
2	6	0	4.040	4.096	-.056
2	8	0	2.552	-1.986	-.565
2	10	0	4.774	-5.043	.270
2	12	0	1.202	-.625	-.578
2	14	0	3.525	3.408	.117
2	16	0	2.142	2.404	-.262
2	18	0	1.078	-1.012	-.066
2	20	0	2.758	-2.980	.222
3	1	0	.430	-.277	-.153
3	3	0	4.139	-4.304	.165
3	5	0	1.333	1.287	.046
3	7	0	.574	-.518	-.056
3	9	0	.836	-.813	-.024
3	11	0	2.656	-2.488	-.168
3	13	0	2.350	2.177	.174
3	15	0	1.613	-1.316	-.297
3	17	0	.060	-.198	.138
3	19	0	.326	.425	-.100
3	21	0	.000	.366	-.366
4	0	0	4.122	4.575	-.453
4	2	0	1.886	1.643	.242
4	4	0	1.291	-1.066	-.225
4	6	0	5.565	-5.818	.253
4	8	0	3.547	3.391	.157
4	10	0	4.239	4.249	-.010
4	12	0	1.653	1.575	.078
4	14	0	3.565	-3.516	-.049
4	16	0	1.190	-1.110	-.080
4	18	0	1.490	1.631	-.141
4	20	0	1.904	1.876	.028
5	1	0	1.225	-1.171	-.054
5	3	0	1.166	-.907	-.259
5	5	0	.569	-.423	-.146

5	7	0	2.170	-1.798	-.372
5	9	0	1.364	.112	.253
5	11	0	2.089	-1.890	-.199
5	13	0	.224	-.183	-.042
5	15	0	.000	-.363	.363
5	17	0	.360	.392	-.032
5	19	0	.311	-.618	.306
6	0	0	3.649	-3.652	.002
6	2	0	4.553	-4.906	.353
6	4	0	1.697	-1.263	-.434
6	6	0	.259	-.104	-.155
6	8	0	3.226	-2.896	-.330
6	10	0	5.613	-5.534	-.079
6	12	0	2.542	-2.431	-.111
6	14	0	.000	-.135	.135
* 6	16	0	.000	-1.135	1.135
6	18	0	1.384	-1.414	.029
6	20	0	2.518	-2.454	-.064
7	1	0	1.726	1.718	.008
7	3	0	.810	.671	.139
7	5	0	.000	.180	-.180
7	7	0	.000	.064	-.064
7	9	0	2.910	2.780	.130
7	11	0	.502	.395	.107
7	13	0	.262	.331	-.069
7	15	0	.000	.004	-.004
7	17	0	.572	.880	-.308
7	19	0	.946	.869	.077
8	0	0	3.980	3.627	.353
8	2	0	.372	.257	.115
8	4	0	.565	-.396	-.169
8	6	0	2.489	-2.051	-.437
8	8	0	2.013	1.794	.219
8	10	0	1.562	1.475	.087
8	12	0	.442	.413	.030
8	14	0	1.160	-.976	-.184
8	16	0	.213	-.502	.288
8	18	0	.906	1.003	-.098
9	1	0	1.407	1.419	-.012
9	3	0	1.325	-1.287	-.038
9	5	0	1.319	-1.246	-.073
9	7	0	.642	-.661	.019
9	9	0	.892	.924	-.032
9	11	0	.000	.027	-.027
9	13	0	.386	-.574	.188
9	15	0	.413	-.676	.263
9	17	0	.000	.017	-.017
10	0	0	3.042	2.978	.064
10	2	0	.743	.707	.036
10	4	0	.445	-.381	-.064
10	6	0	.448	-.360	-.088
10	8	0	1.662	1.596	.067
10	10	0	.838	.895	-.056
10	12	0	.428	-.291	-.137
10	14	0	.000	.227	-.227
10	16	0	.463	-.464	.001
11	1	0	.439	-.153	-.286
11	3	0	1.318	1.348	-.030
11	5	0	2.089	1.989	.100
11	7	0	.457	.400	.057
11	9	0	.234	.130	.104
11	11	0	.491	.411	.081

11	13	0	.261	.656	-.395
11	15	0	.239	.110	.129
12	0	0	.543	.468	.075
12	2	0	1.578	1.624	-.045
12	4	0	4.405	4.512	-.106
12	6	0	2.913	3.052	-.139
12	8	0	1.116	1.231	-.115
12	10	0	.000	.757	-.757
12	12	0	1.081	1.064	.017
12	14	0	2.084	1.925	.159
13	1	0	.000	.009	-.009
13	3	0	1.468	-1.423	-.045
13	5	0	1.556	-1.527	-.029
13	7	0	.626	-.695	.069
13	9	0	.377	-.304	-.073
13	11	0	.503	-.763	.259
13	13	0	1.476	-.432	-1.044
14	0	0	2.541	2.582	-.040
14	2	0	.787	.821	-.035
14	4	0	1.007	-1.219	.212
14	6	0	.879	-1.039	.160
14	8	0	.900	.900	.000
* 14	10	0	.000	1.818	-1.818
14	12	0	.349	.321	.028
15	1	0	1.874	.328	1.546
15	3	0	.000	.405	-.405
15	5	0	.000	.565	-.565
15	7	0	.579	.618	-.039
* 15	9	0	.000	.568	-.568
16	0	0	1.162	-1.124	-.038
16	2	0	.515	-.819	.304
16	4	0	.259	.126	.133
16	6	0	1.123	.429	.694
0	0	1	3.054	3.664	-.610
0	2	1	3.132	3.574	-.142
0	4	1	3.021	-2.604	-.417
0	6	1	2.100	1.671	.430
* 0	8	1	.000	.952	-.952
0	10	1	4.188	4.012	.177
0	12	1	2.183	1.884	.300
0	14	1	.000	.401	-.401
0	16	1	.611	-.497	-.115
0	18	1	1.857	1.753	.105
0	20	1	1.565	1.679	-.114
1	1	1	2.200	-2.145	-.056
1	1	-1	.978	-.805	-.173
1	3	1	1.428	1.247	.181
1	3	-1	1.232	1.089	.142
* 1	5	1	.000	-1.243	1.243
1	5	-1	1.028	-1.091	.062
1	7	1	1.035	-1.047	.013
1	7	-1	.990	.882	.108
1	9	1	.000	-.088	.088
1	9	-1	2.058	-1.781	-.276
1	11	1	.000	.179	-.179
1	11	-1	.000	-.026	.026
1	13	1	1.754	-1.789	.034
1	13	-1	1.129	.999	.130
1	15	1	.000	.117	-.117
1	15	-1	.821	.697	.124
1	17	1	.000	.403	-.403
1	17	-1	1.363	-1.384	.020

1	19	1	.000	-.264	.264
1	19	-1	.545	-.491	-.053
1	21	1	.000	-.608	.608
1	21	-1	.000	.494	-.494
2	0	1	4.977	-5.842	.864
2	0	-1	2.886	-3.036	.150
2	2	1	.691	-.280	-.412
2	2	-1	3.769	-3.802	.034
2	4	1	3.234	2.754	.481
2	4	-1	3.101	-2.939	-.162
2	6	1	4.931	4.926	.006
2	6	-1	4.144	-4.061	-.084
2	8	1	1.085	-.578	-.507
2	8	-1	2.624	-2.329	-.295
2	10	1	4.469	-4.491	.022
2	10	-1	3.451	-3.203	-.248
2	12	1	.923	-.552	-.371
2	12	-1	2.382	-2.104	-.278
2	14	1	3.688	3.415	.273
2	14	-1	2.059	-1.877	-.182
2	16	1	3.063	2.434	.629
2	16	-1	1.206	-1.166	-.040
2	18	1	1.706	-1.645	-.061
2	18	-1	1.875	-1.950	.075
2	20	1	1.139	-.980	-.159
2	20	-1	1.442	-1.369	-.073
2	22	-1	.000	-.949	.949
3	1	1	1.011	-.880	-.131
3	1	-1	1.434	1.224	.210
3	3	1	.736	-.684	-.052
3	3	-1	1.652	1.579	.073
3	5	1	1.900	1.801	.099
3	5	-1	1.390	-1.158	-.232
3	7	1	.604	.554	.050
3	7	-1	1.729	1.481	.248
3	9	1	2.944	-2.668	-.276
3	9	-1	.793	.702	.092
3	11	1	.588	.480	.107
3	11	-1	2.105	2.025	.080
3	13	1	1.475	1.337	.139
3	13	-1	1.089	-1.073	-.016
3	15	1	.000	-.113	.113
3	15	-1	.000	.080	-.080
3	17	1	.666	-.919	.253
3	17	-1	1.208	1.209	-.001
3	19	1	.000	.374	-.374
3	19	-1	.000	.453	-.453
3	21	1	.000	.116	-.116
3	21	-1	.000	-.091	.091
4	0	1	1.640	-1.254	-.386
4	0	-1	3.607	-3.756	.149
4	2	1	5.401	5.614	-.212
4	2	-1	1.808	-1.309	-.499
4	4	1	.451	.468	-.017
4	4	-1	.887	.604	.283
4	6	1	1.242	-1.177	-.065
4	6	-1	.785	.751	.034
4	8	1	.549	-.276	-.273
4	8	-1	1.620	-1.187	-.433
4	10	1	6.549	6.914	-.364
4	10	-1	2.753	-2.482	-.271
4	12	1	2.633	2.554	.079

4	12	-1	1.966	-1.714	-.252
4	14	1	1.014	-1.067	.053
4	14	-1	1.884	1.773	.112
4	16	1	.000	-.228	.228
4	16	-1	.479	-.362	-.117
4	18	1	1.564	1.683	-.118
4	18	-1	.532	-.520	-.011
4	20	1	2.380	2.482	-.102
4	20	-1	.000	-.756	.756
5	1	1	1.226	-1.190	-.036
* 5	1	-1	.000	-2.156	2.156
5	3	1	.644	-.632	-.012
* 5	3	-1	.000	2.209	-2.209
5	5	1	.802	.764	.038
* 5	5	-1	.000	2.477	-2.477
5	7	1	1.286	1.222	.063
* 5	7	-1	.000	1.384	-1.384
5	9	1	1.989	-1.777	-.213
* 5	9	-1	.000	-3.644	3.644
5	11	1	2.315	-2.172	-.142
* 5	11	-1	.000	.254	-.254
5	13	1	.634	.580	.054
* 5	13	-1	.000	2.068	-2.068
5	15	1	1.378	1.454	-.076
* 5	15	-1	.000	.357	-.357
5	17	1	1.147	-1.123	-.024
* 5	17	-1	.000	-1.009	1.009
5	19	1	.000	-.680	.680
* 5	19	-1	.000	-.601	.601
* 5	21	-1	.000	.569	-.569
6	0	1	5.759	-6.272	.514
6	0	-1	2.112	-2.063	-.049
6	2	1	3.821	-.757	-.064
* 6	2	-1	.000	-1.580	1.580
6	4	1	2.617	-2.079	-.538
* 6	4	-1	.000	1.997	-1.997
6	6	1	2.775	2.363	.412
* 6	6	-1	.000	-4.021	4.021
6	8	1	4.084	-3.885	-.199
* 6	8	-1	.000	-2.362	2.362
6	10	1	5.871	-5.926	.055
* 6	10	-1	.000	.566	-.566
6	12	1	1.928	-1.819	-.109
* 6	12	-1	.000	.411	-.411
6	14	1	.766	.609	.157
* 6	14	-1	.000	-2.622	2.622
6	16	1	.564	.689	-.125
* 6	16	-1	.000	-1.793	1.793
6	18	1	1.901	-1.865	-.038
* 6	18	-1	.000	-.702	.702
* 6	20	-1	.000	-.067	.067
7	1	1	2.957	2.965	-.008
* 7	1	-1	.000	.984	-.984
7	3	1	2.251	2.014	.237
* 7	3	-1	.000	1.064	-.1064
7	5	1	1.666	-1.563	-.103
* 7	5	-1	.000	.255	-.255
7	7	1	.510	-.430	-.080
* 7	7	-1	.000	3.091	-3.091
7	9	1	3.970	3.929	.041
* 7	9	-1	.000	.503	-.503
7	11	1	2.618	2.849	-.230

* 7	11	-1	.000	- .974	.974
7	13	1	1.367	-1.371	.004
* 7	13	-1	.000	.678	-.678
7	15	1	.000	.077	-.077
* 7	15	-1	.000	1.692	-1.692
7	17	1	.771	.747	.023
* 7	17	-1	.000	.634	-.634
7	19	1	.000	1.028	-1.028
* 7	19	-1	.000	-.219	.219
8	0	1	1.035	1.075	-.039
8	0	-1	3.685	3.381	.304
8	2	1	.000	-.010	.010
* 8	2	-1	.000	1.937	-1.937
8	4	1	6.393	-6.571	.178
* 8	4	-1	.000	4.169	-4.169
8	6	1	3.446	-3.324	-.121
* 8	6	-1	.000	6.115	-6.115
8	8	1	.533	-.451	-.082
* 8	8	-1	.000	2.720	-2.720
8	10	1	1.345	1.036	.309
* 8	10	-1	.000	-.664	.664
8	12	1	.726	-.505	-.221
* 8	12	-1	.000	1.311	-1.311
8	14	1	1.848	-1.836	-.012
* 8	14	-1	.000	3.587	-3.587
8	16	1	1.961	-2.116	.155
* 8	16	-1	.000	2.216	-2.216
8	18	1	.000	-.313	.313
* 8	18	-1	.000	1.037	-1.037
9	1	1	1.868	-1.706	-.162
* 9	1	-1	.000	-.367	.367
9	3	1	1.767	1.505	.262
* 9	3	-1	.000	-.108	.108
9	5	1	3.947	3.901	.046
* 9	5	-1	.000	-3.076	3.076
9	7	1	.779	.742	.037
* 9	7	-1	.000	-2.756	2.756
9	9	1	3.069	-2.951	-.119
* 9	9	-1	.000	.900	-.900
9	11	1	.000	-.144	.144
* 9	11	-1	.000	.964	-.964
9	13	1	1.366	1.381	-.015
* 9	13	-1	.000	-1.856	1.856
9	15	1	.910	.962	-.052
* 9	15	-1	.000	-1.799	1.799
9	17	1	.000	-.668	.668
* 9	17	-1	.000	.052	-.052
* 9	19	-1	.000	-.575	.575
10	0	1	6.967	-7.615	.648
10	0	-1	5.968	6.416	-.448
10	2	1	2.779	-2.549	-.229
10	2	-1	2.803	2.727	.076
10	4	1	1.135	.929	.206
10	4	-1	.720	-.296	-.424
10	6	1	.000	-.288	.288
10	6	-1	1.228	-.925	-.302
10	8	1	3.702	-3.558	-.144
10	8	-1	3.549	3.176	.372
10	10	1	3.423	-3.448	.026
10	10	-1	3.157	2.881	.276
10	12	1	2.041	-1.987	-.054
10	12	-1	1.741	1.706	.035

10	14	1	.000	.124	-.124
10	14	-1	.350	-.089	-.261
10	16	1	.000	.392	-.392
10	16	-1	.867	-.971	.104
10	18	-1	.000	.179	-.179
11	1	1	2.992	2.887	.105
11	1	-1	2.379	-2.110	-.269
11	3	1	.980	1.138	-.158
11	3	-1	.000	.248	-.248
11	5	1	.000	.398	-.398
11	5	-1	2.856	2.487	.369
11	7	1	2.080	1.926	.155
11	7	-1	.000	.262	-.262
11	9	1	1.828	1.824	.005
11	9	-1	2.735	-2.674	-.062
11	11	1	1.405	1.465	-.060
11	11	-1	.970	-.909	-.060
11	13	1	.000	.499	-.499
11	13	-1	1.619	1.613	.006
11	15	1	.000	.434	-.434
11	15	-1	.000	.388	-.388
11	17	-1	.000	.148	-.148
12	0	1	1.592	1.635	-.043
12	0	-1	2.552	-2.182	-.370
12	2	1	1.189	1.089	.101
12	2	-1	1.167	1.047	.120
12	4	1	.780	-.613	-.167
12	4	-1	5.383	5.431	-.048
12	6	1	.000	.291	-.291
12	6	-1	3.170	2.994	.176
12	8	1	.000	.589	-.589
12	8	-1	.000	.107	-.107
12	10	1	1.442	1.379	.063
12	10	-1	.000	-.422	.422
12	12	1	.000	.811	-.811
12	12	-1	.000	.435	-.435
12	14	-1	2.374	2.041	.332
12	16	-1	2.275	2.193	.083
13	1	1	1.073	-1.181	.108
13	1	-1	.000	-.499	.499
13	3	1	.889	.857	.032
13	3	-1	2.507	-2.235	-.272
13	5	1	.729	1.031	-.301
13	5	-1	2.878	-2.819	-.058
13	7	1	.000	-.147	.147
13	7	-1	1.233	-1.354	.121
13	9	1	1.205	-1.165	-.040
13	9	-1	.000	-.202	.202
13	11	1	.000	-.574	.574
13	11	-1	1.016	-.951	-.065
13	13	-1	.000	-.855	.835
13	15	-1	1.651	-1.506	-.145
14	0	1	.000	-.031	.031
14	0	-1	1.039	.831	.208
14	2	1	.000	.724	-.724
14	2	-1	.804	-.805	.001
14	4	1	.956	1.121	-.164
14	4	-1	1.685	-1.666	-.019
14	6	1	1.162	1.143	.018
14	6	-1	1.626	-1.491	-.135
14	8	1	.000	.193	-.193
14	8	-1	.520	-.489	-.032

14	10	-1	.000	.004	-.004
14	12	-1	.000	.036	-.036
15	1	1	.000	1.132	-1.132
15	1	-1	1.474	-1.529	.055
15	3	1	.000	.324	-.324
15	3	-1	1.293	1.203	.090
15	5	1	.000	.054	-.054
15	5	-1	2.095	2.088	.007
15	7	-1	.000	.198	-.198
15	9	-1	.662	-.775	.113
15	11	-1	.000	-.538	.538
16	0	-1	1.323	-1.446	.123
16	2	-1	.970	-.959	-.011
16	4	-1	.000	.164	-.164
16	6	-1	.000	.063	-.063
16	8	-1	.000	-.701	.701
17	1	-1	.000	.579	-.579
17	3	-1	1.160	-1.205	.045
17	5	-1	1.697	-1.627	-.071
0	0	2	4.602	-5.322	.720
0	2	2	3.450	-3.205	-.245
0	4	2	3.073	2.626	.447
0	6	2	.000	1.331	-1.331
0	8	2	3.088	-2.741	-.347
0	10	2	3.139	-2.769	-.370
0	12	2	1.558	-1.515	-.043
0	14	2	.674	.714	-.040
0	16	2	1.955	1.783	.172
0	18	2	.715	-.706	-.009
0	20	2	1.098	-1.141	.042
1	1	2	.732	-.698	-.034
* 1	1	-2	.000	3.176	-3.176
1	3	2	.480	.148	.332
* 1	3	-2	.000	2.777	-2.777
1	5	2	1.719	1.597	.122
* 1	5	-2	.000	-3.105	3.105
1	7	2	3.494	3.320	.174
* 1	7	-2	.000	1.614	-1.614
1	9	2	3.696	-3.617	-.080
* 1	9	-2	.000	2.436	-2.436
1	11	2	.505	.401	.104
* 1	11	-2	.000	3.618	-3.618
1	13	2	.000	.174	-.174
* 1	13	-2	.000	-2.362	2.362
1	15	2	.973	1.088	-.114
* 1	15	-2	.000	.382	-.382
1	17	2	.424	-.749	.324
* 1	17	-2	.000	.406	-.406
1	19	2	.000	.167	-.167
* 1	19	-2	.000	.843	-.843
1	21	2	.000	.144	-.144
* 1	21	-2	.000	.033	-.033
2	0	2	3.609	-3.376	-.233
2	0	-2	5.302	8.227	-2.925
2	2	2	.823	-.734	-.089
2	2	-2	2.496	-2.233	-.263
2	4	2	1.331	-1.203	-.128
2	4	-2	9.858	-16.404	6.546
2	6	2	2.165	-1.851	-.314
2	6	-2	5.503	-5.797	.294
2	8	2	3.010	-2.733	-.277
2	8	-2	1.029	-.456	-.574

* 2	10	2	.000	.850	-.850
2	10	-2	1.988	1.788	.200
2	12	2	1.268	-1.181	-.086
2	12	-2	3.478	-3.496	.018
2	14	2	1.091	-1.052	-.039
2	14	-2	4.714	-4.835	.121
2	16	2	1.579	-1.666	.087
2	16	-2	4.523	-4.904	.380
2	18	2	.000	-.215	.215
2	18	-2	.379	-.271	-.108
2	20	2	.000	.079	-.079
2	20	-2	.763	.836	-.073
3	1	2	.931	.730	.200
* 3	1	-2	.000	1.572	-1.572
3	3	2	.292	-.154	-.139
* 3	3	-2	.000	4.271	-4.271
5	5	2	2.202	-1.902	-.300
* 3	5	-2	.000	1.607	-1.607
3	7	2	.915	.850	.065
* 3	7	-2	.000	2.457	-2.457
3	9	2	.414	-.267	-.148
* 3	9	-2	.000	.401	-.401
3	11	2	2.066	1.597	.469
* 3	11	-2	.000	3.095	-3.095
3	13	2	1.564	-1.374	-.190
* 3	13	-2	.000	-.907	.907
3	15	2	.000	.076	-.076
* 3	15	-2	.000	1.791	-1.791
3	17	2	.000	.389	-.389
* 3	17	-2	.000	.879	-.879
3	19	2	.000	-.021	.021
* 3	19	-2	.000	.415	-.415
* 3	21	-2	.000	-.213	.213
4	0	2	5.814	6.315	-.502
4	0	-2	7.280	-9.468	2.188
4	2	2	3.196	2.890	.307
4	2	-2	.857	-.036	-.822
4	4	2	.812	.217	.595
4	4	-2	6.701	7.681	-.979
4	6	2	1.988	1.801	.187
4	6	-2	4.188	4.094	.095
4	8	2	4.155	3.732	.423
4	8	-2	3.096	-2.624	-.472
4	10	2	3.894	3.723	.171
4	10	-2	3.512	-3.254	-.258
4	12	2	1.990	1.651	.342
4	12	-2	.618	-.351	-.268
4	14	-2	3.328	3.280	.047
4	14	2	.906	.869	.037
4	16	2	1.794	1.796	-.002
4	16	-2	3.399	3.376	.024
4	18	2	1.456	1.498	-.042
4	18	-2	1.243	-1.141	-.102
4	20	2	1.619	1.720	-.101
4	20	-2	1.152	-1.260	.108
5	1	2	1.023	-.930	-.092
* 5	1	-2	.000	4.454	-4.454
5	3	2	1.413	-1.373	-.040
* 5	3	-2	.000	-1.403	1.403
5	5	2	2.760	-2.639	-.121
* 5	5	-2	.000	-.922	.922
5	7	2	.000	-.051	.051

* 5	7	-2	.000	3.739	-3.739
5	9	2	1.079	-1.049	-.030
* 5	9	-2	.000	-.854	.854
5	11	2	.560	-.590	.029
* 5	11	-2	.000	1.972	-1.972
5	13	2	1.371	-1.211	-.160
* 5	13	-2	.000	.309	-.309
5	15	2	.000	-.541	.541
* 5	15	-2	.000	-.496	.496
5	17	2	.000	-.373	.373
* 5	17	-2	.000	-1.210	1.210
5	19	2	.000	-.093	.093
* 5	19	-2	.000	1.283	-1.283
* 5	21	-2	.000	.400	-.400
6	0	2	2.158	-1.773	-.385
6	0	-2	3.686	3.847	-.160
6	2	2	.000	.058	-.058
6	2	-2	4.806	4.640	.167
6	4	2	1.708	1.616	.092
6	4	-2	5.499	-5.540	.041
6	6	2	2.401	2.032	.569
6	6	-2	3.356	-3.437	.080
6	8	2	1.345	-1.119	-.226
6	8	-2	1.073	.772	.301
6	10	2	.438	-.526	.088
6	10	-2	6.879	7.280	-.401
6	12	2	.000	.331	-.331
6	12	-2	.000	.119	-.119
6	14	2	.713	.740	-.027
6	14	-2	3.794	-3.842	.047
6	16	2	.733	.829	-.096
6	16	-2	1.740	-1.837	.096
6	18	2	.000	-.098	.098
6	18	-2	1.520	1.589	-.069
6	20	-2	1.902	1.956	-.054
7	1	2	.911	.840	.071
* 7	1	-2	.000	-1.230	1.230
7	3	2	.000	-.250	.250
* 7	3	-2	.000	3.722	-3.722
7	5	2	2.106	-1.835	-.271
* 7	5	-2	.000	2.386	-2.386
7	7	2	.000	-.106	.106
* 7	7	-2	.000	1.949	-1.949
7	9	2	1.175	1.154	.021
* 7	9	-2	.000	-.429	.429
7	11	2	.746	.853	-.108
* 7	11	-2	.000	-.234	.234
7	13	2	.631	-.669	.038
* 7	13	-2	.000	-.166	.166
7	15	2	.000	-.034	.034
* 7	15	-2	.000	2.442	-2.442
7	17	2	.000	.371	-.371
* 7	17	-2	.000	.421	-.421
* 7	19	-2	.000	-.416	.416
8	0	2	4.399	4.666	-.267
8	0	-2	2.317	-2.196	-.121
8	2	2	1.423	1.262	.161
8	2	-2	1.576	1.396	.180
8	4	2	3.618	-3.457	-.161
8	4	-2	5.133	5.194	-.060
8	6	2	1.515	-1.443	-.072
8	6	-2	8.186	8.933	-.747

8	8	2	2.641	2.424	.217
8	8	-2	.462	.256	.206
8	10	2	2.274	2.212	.062
8	10	-2	3.669	-3.284	-.386
8	12	2	.515	.516	-.000
* 8	12	-2	.000	2.048	-2.048
8	14	2	1.049	-1.090	.041
8	14	-2	4.534	4.487	.047
8	16	2	.000	-.523	.523
8	16	-2	3.147	3.247	-.101
8	18	-2	.000	-.194	.194
8	20	-2	.000	-.092	.092
9	1	2	2.121	-1.961	-.161
* 9	1	-2	.000	.998	-.998
9	3	2	.000	-.389	.389
* 9	3	-2	.000	-.927	.927
9	5	2	.404	.222	.183
* 9	5	-2	.000	-3.555	3.555
9	7	2	.806	-.726	-.080
* 9	7	-2	.000	-1.055	1.055
9	9	2	1.425	-1.478	.053
* 9	9	-2	.000	1.040	-1.040
9	11	2	.300	-.438	.138
* 9	11	-2	.000	1.005	-1.005
9	13	2	.000	-.547	.547
* 9	13	-2	.000	-2.657	2.657
9	15	2	.000	-.494	.494
* 9	15	-2	.000	-1.452	1.452
* 9	17	-2	.000	-.552	.552
* 9	19	-2	.000	.428	-.428
10	0	2	5.448	-5.698	.250
10	0	-2	2.632	2.644	-.012
10	2	2	2.470	-2.519	.048
* 10	2	-2	.000	2.060	-2.060
10	4	2	1.006	.844	.161
* 10	4	-2	.000	-6.420	6.420
10	6	2	.000	-.128	.128
* 10	6	-2	.000	-3.999	3.999
10	8	2	2.850	-2.609	-.241
* 10	8	-2	.000	1.027	-1.027
10	10	2	3.283	-3.278	-.005
* 10	10	-2	.000	3.523	-3.523
10	12	2	1.772	-1.879	.107
* 10	12	-2	.000	-.942	.942
10	14	2	.000	.058	-.058
* 10	14	-2	.000	-3.036	3.036
* 10	16	-2	.000	-1.494	1.494
* 10	18	-2	.000	.555	-.555
* 11	1	2	.000	1.499	-1.499
11	1	-2	1.345	1.343	.002
* 11	3	2	.000	-.028	.028
11	3	-2	.000	-.089	.089
* 11	5	2	.000	-.292	.292
11	5	-2	.631	.302	.329
* 11	7	2	.000	.876	-.876
11	7	-2	1.443	1.400	.042
* 11	9	2	.000	.887	-.887
11	9	-2	.443	-.212	-.232
* 11	11	2	.000	.778	-.778
11	11	-2	.545	.613	-.068
* 11	13	2	.000	.790	-.790
11	13	-2	.000	.269	-.269

11	15	-2	.562	.703	-.141
11	17	-2	.000	.330	-.330
12	0	2	1.838	2.099	-.260
12	0	-2	3.500	-3.261	-.238
12	2	2	.000	.336	-.336
* 12	2	-2	.000	-1.095	1.095
12	4	2	2.192	-2.172	-.020
* 12	4	-2	.000	-.533	.533
12	6	2	2.027	-2.008	-.019
* 12	6	-2	.000	.071	-.071
* 12	8	2	.000	.399	-.399
* 12	8	-2	.000	-1.414	1.414
12	10	2	1.612	1.634	-.022
* 12	10	-2	.000	-1.792	1.792
* 12	12	-2	.000	-.821	.821
* 12	14	-2	.000	.322	-.322
* 12	16	-2	.000	.622	-.622
* 13	1	2	.000	-.676	.676
* 13	1	-2	.000	-.778	.778
* 13	3	2	.000	-.481	.481
* 13	3	-2	.000	.215	-.215
* 13	5	2	.000	-.508	.508
* 13	5	-2	.000	-.619	.619
* 13	7	2	.000	-.197	.197
* 13	7	-2	.000	-.613	.613
* 13	9	-2	.000	-.429	.429
* 13	11	-2	.000	.336	-.336
* 13	13	-2	.000	-.594	.594
* 13	15	-2	.000	-.768	.768
14	0	2	.000	-.265	.265
14	0	-2	2.812	-2.856	-.044
14	2	2	.000	-.016	.016
* 14	2	-2	.000	-1.901	1.901
14	4	2	.000	.747	-.747
* 14	4	-2	.000	-2.247	2.247
* 14	6	-2	.000	-1.676	1.676
* 14	8	-2	.000	-2.070	2.070
* 14	10	-2	.000	-1.216	1.216
* 14	12	-2	.000	-1.149	1.149
* 14	14	-2	.000	-1.540	1.540
* 15	1	-2	.000	1.222	-.1.222
* 15	3	-2	.000	1.011	-.1.011
* 15	5	-2	.000	1.035	-.1.035
* 15	9	-2	.000	.769	-.769
* 15	7	-2	.000	1.480	-.1.480
* 15	11	-2	.000	.717	-.717
16	0	-2	.428	.265	.162
* 16	2	-2	.000	.039	-.039
* 16	4	-2	.000	-.941	.941
* 16	6	-2	.000	-.547	.547
* 16	8	-2	.000	.208	-.208
* 16	10	-2	.000	.413	-.413
* 17	1	-2	.000	-.271	.271
* 17	3	-2	.000	-.550	.550
* 17	5	-2	.000	-.596	.596
* 17	7	-2	.000	.028	-.028
18	0	-2	.000	.119	-.119
0	0	3	3.141	-3.099	-.043
0	2	3	3.834	-3.660	-.175
0	4	3	5.065	5.721	-.656
0	6	3	5.290	5.394	-.104
0	8	3	1.162	-.735	-.427

0	10	3	6.013	-6.212	.199
0	12	3	1.641	-1.372	-.269
0	14	3	4.162	4.295	-.131
0	16	3	2.145	2.107	.038
0	18	3	1.242	-1.195	-.047
0	20	3	1.499	-2.377	.878
1	1	3	.979	.932	.047
1	1	-3	1.719	-1.510	-.210
1	3	3	2.400	-2.341	-.059
1	3	-3	2.334	2.113	.221
1	5	3	2.465	2.293	.172
1	5	-3	3.442	3.346	.097
1	7	3	.763	-.772	.009
1	7	-3	2.989	-2.890	-.099
1	9	3	.391	-.086	-.305
1	9	-3	2.661	2.387	.273
1	11	3	.000	-.581	.581
1	11	-3	.762	-.803	.041
1	13	3	1.463	1.414	.049
1	13	-3	.000	.341	-.341
1	15	3	.937	-.975	.38
1	15	-3	.542	.279	.264
1	17	3	.000	.117	-.117
1	17	-3	.740	.966	-.227
1	19	3	.000	.145	-.145
1	19	-3	.000	-.481	.481
1	21	-3	.000	.117	-.117
2	0	3	1.301	.809	.492
2	0	-3	6.228	8.953	-2.724
2	2	3	2.826	-2.232	-.594
2	2	-3	2.183	-1.679	-.504
2	4	3	.718	-.861	.143
2	4	-3	2.663	-2.484	-.180
2	6	3	8.576	-9.265	.689
2	6	-3	3.964	-3.731	-.233
2	8	3	1.386	-1.278	-.109
2	8	-3	2.050	1.514	.537
2	10	3	2.686	2.471	.214
2	10	-3	1.936	1.762	.174
2	12	3	.000	-.330	.330
2	12	-3	2.293	1.944	.349
2	14	3	5.011	-4.906	-.105
2	14	-3	3.714	-3.635	-.080
2	16	3	3.233	-3.336	.103
2	16	-3	2.614	-2.719	.105
2	18	3	.000	-.455	.455
2	18	-3	.000	.242	-.242
2	20	3	.000	.347	-.347
2	20	-3	1.373	1.512	-.139
3	1	3	.946	-.776	-.170
3	1	-3	1.562	1.622	-.061
3	3	3	1.368	-1.232	-.136
3	3	-3	1.752	-1.766	.014
3	5	3	2.319	2.213	.106
3	5	-3	2.650	2.442	.208
3	7	3	.000	.022	-.022
3	7	-3	1.136	-1.194	.057
3	9	3	1.336	-1.180	-.156
3	9	-3	1.246	1.274	-.028
3	11	3	1.950	-1.944	-.006
3	11	-3	1.362	-1.352	-.010
3	13	3	2.133	2.077	.055

3	13	-3	1.992	1.961	.031
3	15	-3	.000	.115	-.115
3	17	3	.000	-.470	.470
3	17	-3	.000	-.247	.247
3	19	3	.000	-.777	.777
3	19	-3	.000	-.374	.374
3	21	-3	.000	.434	-.434
4	0	3	1.007	.564	.443
4	0	-3	2.336	2.218	.118
4	2	3	1.779	-.1.385	-.394
4	2	-3	3.758	3.816	-.057
4	4	3	5.373	5.253	.120
4	4	-3	6.354	7.039	-.685
4	6	3	4.770	4.505	.264
4	6	-3	4.623	4.792	-.169
4	8	3	.669	.447	.222
4	8	-3	3.493	3.232	.261
4	10	3	3.172	-2.642	-.530
4	10	-3	2.148	1.718	.430
4	12	3	.858	.754	.104
4	12	-3	1.298	1.191	-.093
4	14	-3	4.140	4.194	-.054
4	14	3	3.277	3.211	.066
4	16	3	1.581	1.693	-.112
4	16	-3	3.532	3.531	.002
4	18	3	.000	.343	-.343
4	18	-3	.761	.900	-.139
4	20	-3	.000	-.704	.704
5	1	3	.839	-.585	-.254
5	1	-3	1.153	1.086	.067
5	3	3	1.751	-.1.616	-.134
5	3	-3	3.711	-3.658	-.053
5	5	3	3.673	-3.538	-.136
5	5	-3	.443	-.211	-.232
5	7	3	3.001	-2.964	-.037
5	7	-3	2.856	-2.716	-.140
5	9	3	2.025	1.914	.111
*5	9	-3	.000	1.208	-.1.208
5	11	3	.000	-.614	.614
5	11	-3	.569	-.786	.216
5	13	3	1.245	-2.083	.838
5	13	-3	.760	-.671	-.089
5	15	3	1.190	-.1.464	.274
5	15	-3	2.051	-2.123	.072
5	17	3	.000	.452	-.452
5	17	-3	.000	.324	-.324
5	19	-3	.000	.180	-.180
5	21	-3	.000	-.494	.494
6	0	3	6.232	6.429	-.197
6	0	-3	4.135	3.677	.457
6	2	3	.870	.756	.115
6	2	-3	.517	.221	.296
6	4	3	.881	-.908	.028
6	4	-3	2.487	1.889	.598
6	6	3	1.369	-.1.117	-.252
6	6	-3	.556	-.341	-.215
6	8	3	3.027	2.761	.266
6	8	-3	1.978	1.631	.347
6	10	3	1.907	1.954	-.048
6	10	-3	1.073	.779	.295
6	12	3	1.151	1.059	.391
6	12	-3	1.778	1.578	.200

6	14	3	.000	-.290	.290
6	14	-3	.590	-.414	-.176
6	16	3	.000	-.931	.931
6	16	-3	.000	-.281	.281
6	18	-3	.000	-.072	.072
6	20	-3	1.088	1.060	.028
7	1	3	2.374	-2.519	.145
7	1	-3	3.614	-3.335	-.279
7	3	3	.000	-.143	.143
7	3	-3	.911	.801	.111
7	5	3	1.755	1.994	-.239
7	5	-3	4.123	3.993	.130
7	7	3	.930	-1.039	.178
7	7	-3	2.102	-1.906	-.196
7	9	3	1.932	-2.071	.139
7	9	-3	2.481	-.2.211	-.270
7	11	3	.515	-.702	.187
7	11	-3	1.835	-1.789	-.046
7	13	3	1.424	1.396	.028
7	13	-3	2.305	2.445	-.140
7	15	3	.000	.120	-.120
7	15	-3	.832	.765	.067
7	17	-3	1.050	-1.193	.142
7	19	-3	.416	-.893	.477
8	0	3	.913	-.259	-.654
8	0	-3	2.336	-2.214	-.122
8	2	3	1.734	1.540	.195
8	2	-3	.656	.427	.230
8	4	3	5.536	5.518	.017
8	4	-3	4.145	3.779	.366
8	6	3	2.984	2.907	.077
8	6	-3	2.361	1.932	.429
8	8	3	1.273	1.237	.037
8	8	-3	2.004	-1.779	-.225
8	10	3	.698	.578	.120
8	10	-3	.618	.559	.059
8	12	3	1.549	1.406	.143
8	12	-3	1.694	1.533	.160
8	14	3	2.615	2.476	.138
8	14	-3	1.179	1.100	.079
8	16	-3	.000	.304	-.304
8	18	-3	.000	.537	-.537
8	20	-3	.000	-.242	.242
9	1	3	1.240	-1.342	.102
9	1	-3	.000	-.140	.140
9	3	3	1.916	-1.884	-.032
9	3	-3	3.205	-2.996	-.209
9	5	3	1.178	-1.179	.001
9	5	-3	2.013	-1.585	-.430
9	7	3	.888	-1.079	.191
9	7	-3	.000	-.392	.392
9	9	3	.784	-.847	.364
9	9	-3	.624	.699	-.075
9	11	3	1.235	-1.223	-.013
9	11	-3	2.370	-2.430	.060
9	13	3	.000	-.488	.488
9	13	-3	1.579	-1.507	-.071
9	15	-3	.000	-.169	.169
9	17	-3	.000	-.087	.087
9	19	-3	.000	-.388	.388
10	0	3	.552	.431	.121
10	0	-3	4.358	-2.058	-2.301

10	2	3	.571	-.625	.054
10	2	-3	4.327	-4.152	-.175
10	4	3	.000	-.261	.261
10	4	-3	3.306	-3.284	-.022
10	6	3	.000	-.525	.525
10	6	-3	1.958	-1.742	-.216
10	8	3	.000	-.078	.078
10	8	-3	1.190	-1.223	.032
10	10	5	.000	-.184	.184
10	10	-3	3.760	-3.798	.038
10	12	3	.000	-.285	.285
10	12	-3	2.358	-2.465	.107
10	14	-3	.965	-.997	.032
10	16	-3	.663	-.803	.141
10	18	-3	1.072	-1.007	-.065
11	1	3	.000	.062	-.062
11	1	-3	.901	.831	.070
11	3	3	.000	.331	-.331
11	3	-3	2.038	1.710	.328
11	5	3	.000	.361	-.361
11	5	-3	1.141	1.133	.008
11	7	3	.000	-.038	.038
11	7	-3	.862	-.817	-.045
11	9	3	.000	.289	-.289
11	9	-3	1.274	1.326	-.352
11	11	-3	2.317	2.191	.127
11	13	-3	.628	.567	.061
* 11	15	-3	.000	.153	-.153
* 11	17	-3	.000	.557	-.557
12	0	3	.000	-.372	.372
12	0	-3	.532	.564	-.032
12	2	3	.000	-.645	.645
12	2	-3	.652	-.690	.038
12	4	3	.000	-.437	.437
12	4	-3	3.288	-3.176	-.112
12	6	3	.000	-.781	.781
12	6	-3	2.860	-2.633	-.227
12	8	3	.000	-.603	.603
12	8	-3	.602	-.625	.023
12	10	-3	.702	.627	.075
12	12	-3	.000	-.385	.385
12	14	-3	.000	-.453	.453
12	16	-3	1.343	-1.448	.106
13	1	3	.000	-.734	.734
* 13	1	-3	.000	-.533	.533
13	3	3	.000	-.339	.339
* 13	3	-3	.000	-.168	.168
* 13	5	-3	.000	1.047	-1.047
* 13	7	-3	.000	.424	-.424
* 13	9	-3	.000	-1.056	1.056
* 13	11	-3	.000	-.487	.487
* 13	13	-3	.000	.620	-.620
* 13	15	-3	.000	.138	-.138
14	0	-3	3.734	-3.999	.265
14	2	-3	1.334	-1.608	.274
14	4	-3	1.330	1.522	-.193
14	6	-3	.856	.144	.712
14	8	-3	1.433	-1.805	.372
14	10	-3	1.415	-1.557	.142
14	12	-3	.755	-.927	.172
14	14	-3	.353	.210	.143
* 15	1	-3	.000	1.613	-1.613

* 15	3	-3	.000	.934	-.934
* 15	5	-3	.000	.485	-.485
* 15	7	-3	.000	.909	-.909
* 15	9	-3	.000	1.243	-1.243
* 15	11	-3	.000	1.134	-1.134
* 15	13	-3	.000	1.005	-1.005
16	0	-3	1.699	1.690	.009
16	2	-3	1.062	.989	.073
16	4	-3	.000	.006	-.006
16	6	-3	.000	.477	-.477
16	8	-3	.000	.663	-.663
16	10	-3	1.366	1.317	.049
16	12	-3	.000	1.246	-1.246
17	1	-3	1.723	-2.191	.468
17	3	-3	.000	.040	-.040
17	5	-3	.000	.835	-.835
17	7	-3	.000	-.494	.494
17	9	-3	1.235	-1.546	.312
18	0	-3	.512	-.475	-.037
* 18	2	-3	.000	.051	-.051
* 18	4	-3	.000	.822	-.822
0	0	4	2.440	-2.300	-.141
0	2	4	1.461	.953	.508
0	4	4	6.313	6.913	-.600
0	6	4	4.172	3.972	.201
0	8	4	.561	-.295	-.267
0	10	4	1.450	-1.260	-.190
0	12	4	.000	2.295	-2.295
0	14	4	3.018	2.952	.066
0	16	4	1.310	1.329	-.019
0	18	4	.000	-.006	.006
1	1	4	1.703	1.453	.251
1	1	-4	.000	-.314	.314
1	3	4	.430	.288	.142
1	3	-4	.000	-.063	.063
1	5	4	1.522	1.374	.148
1	5	-4	1.971	2.012	-.041
1	7	4	.441	-.343	-.097
1	7	-4	.000	.017	-.017
1	9	4	1.491	1.343	.148
1	9	-4	.501	.286	.215
1	11	4	.586	.460	.128
1	11	-4	1.604	-1.509	-.095
1	13	4	.000	.248	-.248
1	13	-4	1.013	1.099	-.086
1	15	4	.000	-.099	.099
1	15	-4	.000	.175	-.175
1	17	4	.000	.499	-.499
1	17	-4	.000	-.183	.183
1	19	4	.000	.068	-.068
1	19	-4	.000	.192	-.192
2	0	4	2.797	2.705	.092
2	0	-4	2.920	3.435	-.514
2	2	4	.511	-.333	-.178
* 2	2	-4	.000	1.551	-1.551
2	4	4	6.900	-7.411	.510
* 2	4	-4	.000	.284	-.284
2	6	4	5.837	-5.971	.134
* 2	6	-4	.000	.916	-.916
2	8	4	.683	.494	.189
* 2	8	-4	.000	1.667	-1.667
2	10	4	2.447	2.181	.265

* 2	10	-4	.000	2.610	-2.610
2	12	4	2.865	-2.690	-.175
* 2	12	-4	.000	-.422	.422
2	14	4	3.661	-3.822	.161
* 2	14	-4	.000	-.613	.613
2	16	4	.000	-2.376	2.376
* 2	16	-4	.000	.418	-.418
2	18	4	.000	.026	-.026
* 2	18	-4	.000	1.461	-1.461
* 2	20	-4	.000	-.269	.269
3	1	4	3.219	3.153	.066
3	1	-4	.728	.639	.089
3	3	4	.000	-.016	.016
3	3	-4	1.498	-1.322	-.176
3	5	4	.509	.455	.054
3	5	-4	2.176	-1.800	-.376
3	7	4	1.673	1.535	.137
3	7	-4	2.294	-2.179	-.115
3	9	4	2.114	1.999	.115
3	9	-4	2.616	2.358	.258
3	11	4	.000	.486	-.486
3	11	-4	.531	-.468	-.063
3	13	4	.000	.710	-.710
3	13	-4	.915	-.963	.048
3	15	4	.521	.184	.337
3	15	-4	1.137	-1.212	.075
3	17	4	.000	.353	-.353
3	17	-4	.000	.483	-.483
3	19	-4	.000	.024	-.024
4	0	4	4.903	-5.096	.192
4	0	-4	7.383	10.789	-3.405
4	2	4	2.435	-2.036	-.399
4	2	-4	2.379	2.042	.338
4	4	4	2.590	2.465	.125
4	4	-4	.952	.166	.786
4	6	4	1.770	1.675	.095
4	6	-4	1.974	1.603	.370
4	8	4	3.364	-2.765	-.599
4	8	-4	5.970	5.927	.043
4	10	4	3.189	-3.020	-.169
4	10	-4	2.664	2.260	.405
4	12	4	.594	-.573	-.020
4	12	-4	2.401	2.409	-.008
4	14	4	.878	1.023	-.144
4	14	-4	1.995	1.677	.318
4	16	4	.872	.909	-.036
4	16	-4	.716	.768	-.052
4	18	-4	1.031	1.003	.028
4	20	-4	1.620	1.923	-.302
5	1	4	.451	.301	.151
5	1	-4	2.394	-2.482	.088
5	3	4	.664	.604	.059
5	3	-4	1.713	-1.934	.221
5	5	4	.590	-.455	-.135
5	5	-4	.443	-.185	-.257
5	7	4	.360	-.511	.150
5	7	-4	3.087	-3.070	-.018
5	9	4	1.220	1.093	.127
5	9	-4	1.067	-.865	-.202
5	11	4	.000	-.077	.077
5	11	-4	1.561	-1.401	-.159
5	13	4	.806	-.646	-.160

5	13	-4	1.125	-•.996	-•.129
5	15	4	.000	.115	-•.115
5	15	-4	1.238	-•.221	-•.017
5	17	4	.000	-•.374	•.374
5	17	-4	.000	.308	-•.308
5	19	-4	.764	-•.737	-•.027
6	0	4	3.279	3.058	•.221
6	0	-4	4.745	-5.053	•.308
6	2	4	.729	-.550	-•.179
* 6	2	-4	.000	-2.374	2.374
6	4	4	5.437	-5.667	•.230
* 6	4	-4	.000	2.788	-2.788
6	6	4	3.127	-2.981	-•.146
* 6	6	-4	.000	-1.249	1.249
6	8	4	.620	.453	•.167
* 6	8	-4	.000	-2.618	2.618
6	10	4	1.152	1.028	•.124
* 6	10	-4	.000	-1.585	1.585
6	12	4	1.064	-.823	-•.241
* 6	12	-4	.000	-2.126	2.126
6	14	4	2.405	-2.231	-•.174
* 6	14	-4	.000	.155	-•.155
6	16	4	2.304	-2.230	-•.075
* 6	16	-4	.000	-.049	•.049
* 6	18	-4	.000	-.361	•.361
* 6	20	-4	.000	-2.018	2.018
7	1	4	.237	.175	•.063
7	1	-4	3.086	2.821	•.266
7	3	4	1.026	.860	•.166
7	3	-4	4.013	-3.963	-•.050
7	5	4	1.286	1.281	•.005
7	5	-4	2.738	-2.373	-•.365
7	7	4	.278	.295	-•.016
7	7	-4	.000	.131	-•.131
7	9	4	.000	.234	-•.234
7	9	-4	1.070	.930	•.140
7	11	4	.618	.650	-•.032
7	11	-4	.000	-.281	•.281
7	13	4	.000	-.083	•.083
7	13	-4	1.093	1.189	-•.096
7	15	4	.000	.378	-•.378
7	15	-4	1.030	-1.527	•.497
7	17	-4	.000	-.601	•.601
7	19	-4	.000	.766	-•.766
8	0	4	1.760	-1.896	•.136
8	0	-4	4.678	4.427	•.251
8	2	4	.836	.811	•.025
8	2	-4	2.048	-1.631	-•.417
8	4	4	3.266	3.238	•.028
8	4	-4	1.794	-1.593	-•.201
8	6	4	2.357	2.480	-•.123
8	6	-4	5.355	-5.229	-•.126
8	8	4	.000	.458	-•.458
8	8	-4	.989	.768	•.221
8	10	4	.000	-.415	•.415
8	10	-4	2.989	2.776	•.213
8	12	4	.000	.078	-•.078
8	12	-4	.758	.752	•.006
8	14	-4	3.054	-3.184	•.130
8	16	-4	1.338	-1.397	•.059
8	18	-4	.000	.800	-•.800
9	1	4	.000	.163	-•.163

9	1	-4	4.480	-4.573	.093
9	3	4	1.149	-1.111	-.038
9	3	-4	1.166	.979	.188
9	5	4	.957	-1.023	.066
9	5	-4	2.632	2.443	.189
9	7	4	.000	-.285	.285
9	7	-4	.963	-1.160	.198
9	9	4	.000	-.481	.481
9	9	-4	1.521	-1.478	-.043
9	11	4	.000	-.124	.124
9	11	-4	2.834	-2.711	-.123
9	13	4	.000	.089	-.089
9	15	-4	1.450	1.338	.112
9	17	4	.000	.546	-.546
9	19	-4	1.279	-1.398	.120
10	0	4	1.086	1.641	-.556
10	0	-4	4.868	-4.975	.106
10	2	4	.919	.809	.111
*10	2	-4	.000	-5.156	5.156
10	4	4	.950	-.961	.011
*10	4	-4	.000	1.309	-1.309
10	6	4	.649	-.921	.272
*10	6	-4	.000	2.687	-2.687
10	8	4	.000	.445	-.445
*10	8	-4	.000	-2.955	2.955
*10	10	4	.000	-6.602	6.602
*10	12	-4	.000	-1.861	1.861
*10	14	4	.000	2.070	-2.070
*10	16	-4	.000	-.326	.326
*10	18	4	.000	-1.310	1.310
11	1	4	.000	.515	-.515
11	1	-4	3.343	3.315	.027
11	3	4	.000	.522	-.522
11	3	-4	.307	-.499	.193
11	5	4	.000	.352	-.352
11	5	-4	2.110	-1.890	-.219
11	7	4	.596	-.382	-.214
11	9	-4	3.919	3.893	.027
11	11	4	1.808	2.368	-.560
11	13	-4	.000	-.380	.380
11	15	4	1.054	-1.156	.102
11	17	-4	1.328	1.315	.013
12	0	-4	6.400	7.227	-.826
12	2	-4	2.065	1.826	.240
12	4	-4	2.619	-2.399	-.220
12	6	-4	4.172	-3.802	-.370
12	8	-4	4.140	4.029	.111
12	10	-4	4.567	4.716	-.149
12	12	-4	.000	.579	-.579
12	14	-4	2.018	-1.895	-.123
12	16	-4	.000	-.427	.427
13	1	-4	1.508	-1.408	-.099
13	3	-4	1.537	-1.663	.126
13	5	-4	.696	.413	.283
13	7	-4	.000	-.061	.061
13	9	-4	1.795	-1.708	-.087
13	11	-4	1.649	-1.835	.186
13	13	-4	.000	.451	-.451
13	15	-4	.000	.069	-.069
14	0	-4	.378	-1.213	.835
*14	2	-4	.000	.018	-.018
*14	4	-4	.000	3.469	-3.469

*14	6	-4	.000	2.215	-2.215
*14	8	-4	.000	-.256	.256
*14	10	-4	.000	-.961	.961
*14	12	-4	.000	.279	-.279
*14	14	-4	.000	1.788	-1.788
15	1	-4	.000	.632	-.632
15	3	-4	.000	.011	-.011
15	5	-4	1.038	-1.168	.130
15	7	-4	.949	-1.070	.120
15	9	-4	1.122	1.306	-.183
15	11	-4	.714	.974	-.260
15	13	-4	.000	.038	-.038
16	0	-4	3.080	3.030	.050
16	2	-4	1.313	1.347	-.034
16	4	-4	.737	.590	.147
16	6	-4	.000	.280	-.280
16	8	-4	1.501	1.532	-.031
16	10	-4	1.714	1.784	-.070
16	12	-4	1.269	1.209	.060
17	1	-4	1.973	-2.206	.233
17	3	-4	1.177	-1.243	.066
17	5	-4	.000	-.152	.152
17	7	-4	.831	-.914	.083
17	9	-4	1.763	-1.845	.082
18	0	-4	.628	-.519	-.109
*18	2	-4	.000	-.289	.289
*18	4	-4	.000	.425	-.425
*18	6	-4	.000	.206	-.206
0	0	5	1.531	1.680	-.149
0	2	5	6.166	6.383	-.217
0	4	5	.580	.597	-.017
0	6	5	.782	-.821	.038
0	8	5	1.698	1.639	.059
0	10	5	6.206	6.561	-.354
0	12	5	2.011	2.598	-.586
0	14	5	.000	-.398	.398
0	16	5	.000	.197	-.197
0	18	5	1.651	1.586	.064
1	1	5	.465	.365	.099
1	1	-5	.302	-.171	-.131
1	3	5	.712	.706	.006
1	3	-5	.292	.129	.163
1	5	5	.000	.080	-.080
1	5	-5	1.090	-.162	.073
1	7	5	1.728	1.671	.057
1	7	-5	1.765	1.957	-.192
1	9	5	2.068	-1.895	-.173
1	9	-5	1.880	-1.847	-.033
1	11	5	.000	.545	-.545
1	11	-5	.000	.423	-.423
1	13	5	.845	.707	.138
1	13	-5	.530	-.690	.161
1	15	5	.000	.737	-.737
1	15	-5	.000	.180	-.180
1	17	5	1.213	-.184	-.029
1	17	-5	.000	-.346	.346
1	19	-5	.000	.340	-.340
2	0	5	3.588	-.525	-.063
2	0	-5	5.902	-6.590	.688
2	2	5	.000	-.172	.172
2	2	-5	1.749	-1.651	-.097
2	4	5	.603	.438	.165

2	4	-5	2.106	1.885	.221
2	6	5	2.413	2.005	.408
2	6	-5	5.641	5.437	.204
2	8	5	1.543	-1.457	-.086
2	8	-5	2.264	-1.851	-.413
2	10	5	2.403	-2.247	-.157
2	10	-5	5.733	-5.806	.073
2	12	5	.000	-.341	.341
2	12	-5	1.397	-1.417	.020
2	14	5	.738	.635	.103
2	14	-5	2.993	2.925	.068
2	16	5	.000	.424	-.424
2	16	-5	2.028	2.092	-.064
2	18	-5	1.894	-1.786	-.108
3	1	5	1.455	1.467	-.012
3	1	-5	5.485	-5.512	.027
3	3	5	2.284	2.333	-.049
3	3	-5	3.863	3.942	-.079
3	5	5	.000	-.055	.55
3	5	-5	.702	-.763	.062
3	7	5	1.607	1.654	-.047
3	7	-5	.884	-.698	-.186
3	9	5	1.653	1.543	.110
3	9	-5	1.532	-1.533	.001
3	11	5	1.099	1.333	-.234
3	11	-5	.994	1.214	-.221
3	13	5	.000	-.652	.652
3	13	-5	.954	-1.310	.356
3	15	5	.000	.836	-.836
3	15	-5	.706	.726	-.021
3	17	5	.000	.925	-.925
3	17	-5	.000	-.605	.605
3	19	-5	.000	-.400	.400
4	0	5	.478	.613	-.136
4	0	-5	2.517	2.812	-.295
4	2	5	.726	.577	.149
4	2	-5	2.948	2.590	.358
4	4	5	2.491	-2.238	-.254
4	4	-5	6.113	-.6.616	.503
4	6	5	.478	.254	.224
4	6	-5	1.713	-1.917	.204
4	8	5	.000	.154	-.154
4	8	-5	.328	-.090	-.238
4	10	5	.000	.104	-.104
4	10	-5	3.625	3.802	-.178
4	12	5	.278	-.173	-.105
4	12	-5	1.308	1.281	.027
4	14	5	.000	-.083	.083
4	14	-5	1.781	-1.893	.112
4	16	5	.000	.140	-.140
4	16	-5	2.333	-2.629	.296
4	18	-5	1.262	1.152	.110
5	1	5	.000	.062	-.062
5	1	-5	.268	.197	.071
5	3	5	1.361	1.330	.031
5	3	-5	.852	-.770	-.082
5	5	5	.833	.730	.104
5	5	-5	1.730	-1.761	.032
5	7	5	.000	.463	-.463
5	7	-5	2.422	2.288	.134
5	9	5	.000	-.613	.613
5	9	-5	1.956	-1.881	-.075

5	11	5	.000	.708	-.708
5	11	-5	.421	.122	.298
5	13	5	.000	.430	-.430
5	13	-5	.724	-.830	.106
* 5	15	5	.000	.157	-.157
5	15	-5	.676	.841	-.165
5	17	-5	.000	-.539	.539
5	19	-5	.000	-.223	.223
6	0	5	3.824	-3.551	-.273
6	0	-5	7.861	-1.430	2.568
6	2	5	1.927	-1.714	-.213
6	2	-5	3.507	-3.666	.159
6	4	5	1.914	-1.708	-.206
6	4	-5	1.666	-1.098	-.567
6	6	5	1.988	-1.858	-.130
6	6	-5	2.109	-1.875	-.233
6	8	5	2.631	-2.413	-.218
6	8	-5	3.882	-3.646	-.237
6	10	5	1.680	-1.642	-.038
6	10	-5	5.046	-5.171	.125
6	12	5	1.161	-1.040	-.122
6	12	-5	4.244	-4.290	.046
6	14	-5	.000	-.313	.313
6	16	-5	1.502	1.380	.122
6	18	-5	2.523	-2.585	.062
7	1	5	.000	.090	-.090
7	1	-5	2.744	2.417	.327
7	3	5	1.120	1.316	-.196
7	3	-5	1.056	1.017	.040
7	5	5	1.634	1.678	-.044
7	5	-5	.856	-1.026	.170
7	7	5	.000	1.117	-.117
7	7	-5	2.143	2.171	-.027
7	9	5	.000	-.290	.290
7	9	-5	.544	.380	.164
7	11	5	.000	.395	-.395
7	11	-5	3.007	3.023	-.016
7	13	-5	.000	.167	-.167
7	15	-5	.000	-.058	.058
7	17	-5	.000	.134	-.134
7	19	-5	1.483	1.532	-.048
8	0	5	1.383	-1.248	-.135
8	0	-5	.266	.447	-.181
8	2	5	.000	-.092	.092
8	2	-5	1.919	1.416	.503
8	4	5	.000	.532	-.532
8	4	-5	4.626	-4.424	-.203
8	6	5	1.023	.825	.198
8	6	-5	1.741	-1.634	-.107
8	8	5	.000	-.235	.235
8	8	-5	1.556	-1.389	-.166
8	10	5	1.081	-.896	-.185
8	10	-5	2.900	2.650	.250
8	12	-5	1.060	.868	.192
8	14	-5	1.660	-1.356	-.303
8	16	-5	1.999	-2.019	.020
8	18	-5	.000	.548	-.548
9	1	5	.000	.146	-.146
9	1	-5	2.883	-2.957	.073
9	3	5	.848	-.762	-.086
9	3	-5	3.191	3.155	.035
9	5	5	1.229	-1.297	.368

9	5	-5	.000	2.156	-2.156
9	7	5	.000	-.434	.434
9	7	-5	.000	.425	-.425
9	9	-5	2.280	-2.436	.155
9	11	-5	.000	-.221	.221
9	13	-5	1.074	1.092	-.019
9	15	-5	1.941	2.005	-.064
9	17	-5	.601	-.870	.269
10	0	5	1.237	1.061	.177
10	0	-5	5.354	-5.136	-.218
* 10	2	5	.000	.676	-.676
10	2	-5	1.562	-1.336	-.227
10	4	-5	2.576	2.427	.149
10	6	-5	2.461	2.107	.353
10	8	-5	2.659	-2.432	-.227
10	10	-5	3.134	-3.067	-.067
10	12	-5	.000	.324	-.324
10	14	-5	.000	.844	-.844
10	16	-5	.000	.835	-.835
10	18	-5	.000	-.981	.981
11	1	-5	2.404	2.254	.150
11	3	-5	.438	-.293	-.145
11	5	-5	.898	-.855	-.044
11	7	-5	2.202	2.327	-.125
11	9	-5	1.826	1.664	.162
11	11	-5	.664	.845	-.181
11	13	-5	.809	-.863	.054
11	15	-5	.000	.655	-.655
11	17	-5	.000	.929	-.929
12	0	-5	2.650	2.647	.004
12	2	-5	3.192	3.034	.158
12	4	-5	.655	-.260	-.395
12	6	-5	2.079	1.997	.082
12	8	-5	2.635	2.689	-.054
12	10	-5	2.193	2.210	-.017
12	12	-5	.000	.551	-.551
12	14	-5	1.028	1.039	-.010
12	16	-5	.893	.863	.029
13	1	-5	2.354	-2.353	-.000
13	3	-5	.000	-.166	.166
13	5	-5	.000	-.429	.429
13	7	-5	1.968	-1.756	-.212
13	9	-5	2.191	-2.233	.042
13	11	-5	.000	-.224	.224
13	13	-5	.000	-.480	.480
13	15	-5	.000	-.707	.707
14	0	-5	1.003	1.111	-.108
14	2	-5	.000	.755	-.755
14	4	-5	.000	-.176	.176
14	6	-5	.000	-.107	.107
14	8	-5	.000	.350	-.350
14	10	-5	.000	.370	-.370
14	12	-5	.000	.504	-.504
14	14	-5	.000	.044	-.044
15	1	-5	.525	.669	-.144
15	3	-5	.000	-.323	.323
15	5	-5	.672	-.717	.045
15	7	-5	.000	.469	-.469
15	9	-5	.000	.321	-.321
15	11	-5	.000	.112	-.112
15	13	-5	.000	-.235	.235
16	0	-5	1.341	-1.389	.048

16	2	-5	.000	.323	-.323
16	4	-5	.000	1.248	-1.248
16	6	-5	.000	.652	-.652
16	8	-5	.000	-.567	.567
16	10	-5	.000	-.122	.122
16	12	-5	.000	-.001	.001
17	1	-5	.930	-.963	.033
17	3	-5	.000	-.310	.310
17	5	-5	.000	-.295	.295
17	7	-5	.641	-.856	.215
17	9	-5	1.173	-1.260	.087
18	0	-5	.000	-.253	.253
18	2	-5	.000	-.529	.529
18	4	-5	.000	-.799	.799
18	6	-5	.000	-.748	.748
18	8	-5	.000	-.697	.697
*19	1	-5	.000	.370	-.370
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0	2	6	3.276	3.321	-.045
0	4	6	2.405	-2.117	-.288
0	6	6	3.112	-2.867	-.245
0	8	6	3.136	4.659	-1.523
0	10	6	4.470	4.863	-.393
0	12	6	1.043	1.173	-.129
0	14	6	1.526	-1.537	.010
0	16	6	.000	.044	-.044
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1	1	-6	2.217	-2.100	-.117
1	3	6	3.127	-2.965	-.162
1	3	-6	.000	-.188	.188
1	5	6	2.855	-2.743	-.112
1	5	-6	.000	-.290	.290
1	7	6	.000	-.071	.071
1	7	-6	1.231	-1.075	-.156
1	9	6	.000	-.202	.202
1	9	-6	1.696	-1.501	-.194
1	11	6	.701	-.762	.062
1	11	-6	.000	-.475	.475
1	13	6	.635	-.704	.069
1	13	-6	.000	-.164	.164
1	15	6	1.487	-1.303	-.184
1	15	-6	.000	-.303	.303
1	17	-6	.000	.081	-.081
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2	0	-6	6.802	-8.064	1.262
2	2	6	.000	.023	-.023
2	2	-6	3.666	-3.480	-.186
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2	6	6	2.810	2.561	.249
2	6	-6	1.892	1.605	.287
2	8	6	.000	-.318	.318
2	8	-6	4.787	-4.560	-.227
2	10	6	1.434	-.1437	.003
2	10	-6	5.583	-.5786	.203
2	12	6	.000	.313	-.313
2	12	-6	.000	-.509	.509
2	14	6	1.380	1.328	.052
2	14	-6	1.442	1.302	.140
2	16	-6	.000	-.461	.461
2	18	-6	2.242	-1.873	-.369

5	1	6	.597	-.638	.041
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3	3	6	.000	.591	-.591
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3	5	6	.389	-.265	-.125
*3	5	-6	.000	-.1749	1.749
3	7	6	.432	-.417	-.015
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3	9	6	.300	.417	-.417
*3	9	-6	.000	.742	-.742
3	11	6	.382	-.296	-.086
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3	13	6	.000	.060	-.060
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3	15	6	.000	.124	-.124
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*3	17	-6	.000	-.021	.021
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4	2	6	2.167	2.046	.121
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4	4	6	.000	-.175	.175
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4	6	6	.000	.673	-.673
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4	8	6	2.854	2.733	.120
4	8	-6	2.269	2.009	.261
4	10	6	2.421	2.271	.150
4	10	-6	2.266	1.973	.293
4	12	6	1.985	1.951	.034
4	12	-6	.435	-.429	-.006
4	14	-6	3.446	-3.380	-.065
4	16	-6	.000	-.297	.297
4	18	-6	1.336	1.184	.153
5	1	6	.635	-.577	-.059
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5	3	6	.000	-.063	.063
5	3	-6	.802	.667	.135
*5	5	6	.000	.013	-.013
*5	5	-6	.000	.363	-.363
5	9	6	.000	-.058	.058
5	9	-6	.488	-.273	-.215
5	7	6	.828	-.534	-.294
5	7	-6	1.051	.760	.291
5	11	6	.000	-.208	.208
5	11	-6	.000	.138	-.138
5	13	-6	.000	.169	-.169
5	15	-6	.559	.440	.119
5	17	-6	.000	.486	-.486
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6	0	-6	4.144	-4.486	.342
6	2	6	1.053	-.928	-.125
6	2	-6	2.000	-1.629	.371
6	4	6	.000	.338	-.338
6	4	-6	2.650	-2.420	-.230
6	6	6	.000	-.269	.269
6	6	-6	.000	.012	-.012
6	8	6	.000	-.504	.304
6	8	-6	1.897	-1.759	-.139
6	10	6	1.399	-1.379	-.020
6	10	-6	4.024	-3.778	-.247
6	12	-6	2.142	-1.861	-.281

6	14	-6	1.171	1.034	.137
6	16	-6	.000	-.672	.672
6	18	-6	2.001	-1.938	-.063
*	7	1	.000	1.108	-1.108
7	1	-6	1.792	1.672	.120
*	7	3	.000	.098	-.098
7	3	-6	1.449	1.400	.049
*	7	5	.000	.313	-.313
7	5	-6	.000	-.041	.041
*	7	7	.000	.540	-.540
7	7	-6	.950	.900	.051
7	9	-6	1.774	1.665	.109
7	11	-6	2.055	1.954	.101
7	13	-6	.000	.020	-.020
7	15	-6	.000	-.102	.102
7	17	-6	.000	1.127	-1.127
8	0	6	.000	.182	-.182
8	0	-6	1.536	1.925	-.389
8	2	6	.000	-.091	.091
8	2	-6	2.902	2.566	.336
8	4	-6	1.107	.969	.138
8	4	6	.000	-.133	.133
8	6	-6	.839	-.449	-.390
8	8	-6	2.451	2.162	.289
8	10	-6	3.256	3.028	.228
8	12	-6	1.194	1.423	-.228
8	14	-6	.826	-.977	.151
8	16	-6	1.260	1.357	-.097
8	18	-6	1.746	1.590	.156
*	9	1	-6	.000	1.182
*	9	3	-6	.000	-1.387
*	9	5	-6	.000	1.980
*	9	7	-6	.000	-.737
*	9	9	-6	.000	-.401
*	9	11	-6	.000	-.481
*	9	13	-6	.000	.386
*	9	15	-6	.000	-.206
*	9	17	-6	.000	1.312
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10	4	-6	.396	.121	
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10	8	-6	1.002	-.936	
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10	12	-6	.890	.944	
10	14	-6	.000	.032	
10	16	-6	.000	-.542	
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11	5	-6	2.070	2.103	
11	7	-6	.451	.148	
11	9	-6	1.053	-.964	
11	11	-6	.763	-.604	
11	13	-6	.000	-.238	
11	15	-6	1.164	1.256	
11	17	-6	.000	.535	
12	0	-6	.341	-.198	
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12	4	-6	2.045	1.970	
12	6	-6	3.765	3.763	
12	8	-6	1.161	1.151	
12	10	-6	1.952	-1.936	

12	12	-6	.000	.527	-.527
12	14	-6	2.065	2.070	-.005
12	16	-6	1.190	1.296	-.106
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13	3	-6	1.716	-1.685	-.031
13	5	-6	3.413	-3.288	-.125
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13	9	-6	.000	.538	-.538
13	11	-6	.557	.568	-.011
13	13	-6	2.111	-2.045	-.065
13	15	-6	1.943	-1.810	-.133
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14	4	-6	3.928	-4.018	.090
14	6	-6	3.044	-3.094	.049
14	8	-6	.000	.233	-.233
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14	14	-6	2.187	-2.147	-.040
*15	1	-6	.000	.497	-.497
*15	3	-6	.000	.973	-.973
*15	5	-6	.000	2.108	-2.108
*15	7	-6	.000	2.040	-2.040
*15	9	-6	.000	-.474	.474
*15	11	-6	.000	-.351	.351
*15	13	-6	.000	.951	-.951
16	0	-6	2.359	-2.573	.214
16	2	-6	.836	-.802	-.034
16	4	-6	1.272	1.155	.117
16	6	-6	1.093	.710	.382
16	8	-6	1.367	-1.375	.008
16	10	-6	1.457	-1.537	.079
16	12	-6	.000	-.319	.319
17	1	-6	1.360	1.517	-.157
17	3	-6	.000	.480	-.480
17	5	-6	1.282	-1.339	.058
17	7	-6	.000	-.664	.664
17	9	-6	1.255	1.233	.022
18	0	-6	.803	.788	.015
18	2	-6	.000	-.067	-.067
18	4	-6	1.466	-1.732	.266
18	6	-6	.000	-1.054	1.054
18	8	-6	.000	-.194	.194
*19	1	-6	.000	.170	-.170
*19	3	-6	.000	1.777	-1.777
0	0	7	.404	.288	.116
0	2	7	.000	-.500	.500
0	4	7	.000	-.042	.042
0	6	7	.000	-.639	.639
* 0	8	7	.000	-.062	.062
* 0	10	7	.000	.251	-.251
0	12	7	.000	.171	-.171
0	14	7	.000	.030	-.030
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1	3	7	.892	-1.013	.122
1	3	-7	.982	-1.143	.161
1	5	7	.000	-.027	.027
1	5	-7	.000	-.010	.010
1	7	7	.865	-1.056	.191
1	7	-7	.554	-.632	.078
1	9	7	.415	-.479	.065

1	9	-7	.000	.274	-.274
1	11	7	1.076	-1.102	.026
*1	11	-7	.000	-.170	.170
1	13	7	.000	-.493	.493
1	13	-7	.956	.918	.039
1	15	-7	.000	-.238	.238
2	0	7	1.110	-.986	-.123
2	0	-7	1.801	-1.818	.017
2	2	7	1.496	-1.409	-.087
2	2	-7	2.823	-2.567	-.256
2	4	7	.402	.444	-.042
2	4	-7	1.270	-1.349	.079
2	6	7	.000	.655	-.655
2	6	-7	4.311	-4.199	-.112
2	8	7	.000	-.454	.454
2	8	-7	2.199	-2.159	-.041
2	10	7	1.848	-1.679	-.169
2	10	-7	.533	-.521	-.012
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2	12	-7	.891	-1.062	.171
2	14	-7	2.134	-2.085	-.049
2	16	-7	1.476	-1.460	-.015
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3	3	7	.000	-.539	.539
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3	9	7	.000	.254	-.254
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3	11	7	.000	-.207	.207
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4	8	7	1.639	1.465	.174
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4	10	-7	2.555	-2.354	-.201
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5	3	7	.000	.027	-.027
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5	5	7	.717	.765	-.048
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5	7	7	.000	-.711	.711
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7	5	7	.712	.644	.067
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8	10	7	.000	.379	-.379
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9	5	7	1.820	-1.981	.162
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9	9	7	.447	-.308	-.139
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9	13	7	.000	.152	-.152
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10	4	7	1.496	-1.247	-.249
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10	10	-7	1.738	1.763	-.025
10	12	7	1.821	1.873	-.048
10	14	-7	2.006	-2.004	-.002
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11	13	-7	.000	.684	-.684
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12	2	7	1.114	-1.052	-.063
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12	8	-7	1.050	-1.034	-.016

12	10	-7	2.644	-2.716	.072
12	12	-7	.000	-.336	.336
12	14	-7	2.251	2.127	.124
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13	5	-7	1.354	-1.303	-.050
13	7	-7	.000	-.323	.323
13	9	-7	.869	.871	-.002
13	11	-7	.000	-.439	.439
13	13	-7	.000	-.753	.753
14	0	-7	1.511	1.488	.023
14	2	-7	1.145	-1.120	-.025
14	4	-7	2.006	-2.026	.020
14	6	-7	2.929	-2.886	-.043
14	8	-7	.776	.563	.214
14	10	-7	.000	.166	-.166
14	12	-7	.850	-.997	.147
15	1	-7	.000	.341	-.341
15	3	-7	1.996	2.181	-.185
15	5	-7	2.809	3.007	-.198
15	7	-7	1.005	.991	.014
15	9	-7	.000	.278	-.278
15	11	-7	.000	.555	-.555
16	0	-7	.000	.247	-.247
16	2	-7	.000	.010	-.010
16	4	-7	.429	.663	-.234
16	6	-7	.000	.731	-.731
16	8	-7	.000	.076	-.076
16	10	-7	.000	-.160	.160
17	1	-7	1.346	1.241	.105
17	3	-7	.666	-.620	-.045
17	5	-7	1.383	-1.291	-.092
17	7	-7	.000	-.181	.181
17	9	-7	1.121	1.320	-.199
18	0	-7	.000	.264	-.264
18	2	-7	.000	.163	-.163
18	4	-7	.000	.672	-.672
18	6	-7	.000	-.233	.233
19	1	-7	.000	-.390	.390
19	3	-7	.000	.878	-.878
0	0	8	2.403	-2.553	.150
0	2	8	.583	-.698	.114
0	4	8	.287	.258	.030
0	6	8	.578	.531	.047
0	8	8	.902	-.892	-.010
0	10	8	.765	-.700	-.064
0	12	8	.000	-.923	.923
1	1	8	.000	-.076	.076
1	1	-8	2.227	2.399	-.171
1	3	8	.517	.535	-.018
1	3	-8	.000	-.631	.631
1	5	8	.000	-.010	.010
1	5	-8	.000	-.154	.154
1	7	8	.000	.098	-.098
1	7	-8	1.241	1.709	-.467
1	9	8	.000	.109	-.109
1	9	-8	.832	.858	-.026
1	11	-8	.567	.877	-.310
1	13	-8	.000	.081	-.081
2	0	8	1.355	-1.198	-.157
2	0	-8	1.128	1.074	.054
* 2	2	8	.000	-1.583	1.583

2	2	-8	.000	.298	-.298	
*	2	4	.000	-2.638	2.638	
2	4	-8	3.866	-3.787	-.079	
*	2	6	.000	-1.370	1.370	
2	6	-8	3.024	-2.966	-.058	
*	2	8	.000	-1.850	1.850	
2	8	-8	.000	-.292	.292	
2	10	-8	1.848	1.843	.006	
2	12	-8	1.017	-.913	-.104	
3	1	8	.000	-.303	.303	
3	1	-8	.000	-.352	.352	
3	3	8	.000	.441	-.441	
3	3	-8	.000	1.632	-1.632	
3	5	8	.000	.198	-.198	
3	5	-8	1.676	1.727	-.051	
3	7	8	.000	.024	-.024	
3	7	-8	.000	.238	-.238	
3	9	-8	.000	-.452	.452	
3	11	-8	.784	.824	-.040	
3	13	-8	.000	.390	-.390	
4	0	8	.205	.378	-.173	
4	0	-8	1.360	-1.347	-.012	
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*	4	2	-8	.000	.617	-.617
4	4	8	.000	-.329	.329	
*	4	4	-8	.000	4.313	-4.313
*	4	6	-8	.000	4.958	-4.958
*	4	8	-8	.000	-.608	.608
*	4	10	-8	.000	-1.290	1.290
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*	4	14	-8	.000	2.876	-2.876
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5	7	-8	.000	-.277	.277	
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5	11	-8	.000	.408	-.408	
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6	10	-8	3.473	3.375	.098	
6	12	-8	.000	-.531	.531	
6	14	-8	2.163	-1.897	-.265	
7	1	-8	.976	-1.467	.491	
7	3	-8	.000	-.111	.111	
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7	7	-8	.000	.355	-.355	
7	9	-8	.000	-2.215	2.215	
7	11	-8	.000	-.714	.714	
7	13	-8	.000	.286	-.286	
7	15	-8	.000	.744	-.744	
8	0	-8	1.700	-1.553	-.148	
8	2	-8	.000	.221	-.221	
8	4	-8	3.338	3.347	-.008	
8	6	-8	3.196	3.065	.131	
8	8	-8	.000	.199	-.199	
8	10	-8	2.003	-1.810	-.193	
8	12	-8	.000	.159	-.159	

8	14	-8	2.891	2.714	.176
9	1	-8	.909	.946	-.037
9	3	-8	1.299	-1.378	.079
9	5	-8	2.372	-2.874	.502
9	7	-8	.962	-1.076	.114
9	9	-8	.662	.947	-.285
9	11	-8	.665	.683	-.019
* 9	13	-8	.000	-1.918	1.918
* 9	15	-8	.000	-1.755	1.755
10	0	-8	1.295	1.365	-.069
10	2	-8	.256	-.150	-.106
10	4	-8	3.855	-4.128	.273
10	6	-8	2.840	-3.014	.174
10	8	-8	.659	-.671	.012
10	10	-8	2.105	2.025	.080
10	12	-8	1.077	-1.234	.158
10	14	-8	3.219	-3.105	-.113
11	1	-8	.713	.812	-.100
11	3	-8	1.001	.977	.024
11	5	-8	1.640	1.469	.171
11	7	-8	2.081	1.403	.678
11	9	-8	.000	-.136	.136
11	11	-8	.000	-.196	.196
11	13	-8	1.521	1.456	.065
12	0	-8	1.903	-1.901	-.002
*12	2	-8	.000	-.588	.588
*12	4	-8	.000	2.221	-.221
*12	6	-8	.000	.581	-.581
*12	8	-8	.000	-1.287	1.287
*12	10	-8	.000	-1.414	1.414
*12	12	-8	.000	.910	-.910
13	1	-8	.000	-.105	.105
13	3	-8	.725	.775	-.050
13	5	-8	.000	.609	-.609
13	7	-8	.000	-.087	.087
13	9	-8	.000	.272	-.272
13	11	-8	.000	.486	-.486
13	13	-8	.000	-.458	.458
14	0	-8	.000	.035	-.035
14	2	-8	.000	-.455	.455
14	4	-8	1.392	-1.363	-.029
14	6	-8	.000	.389	-.389
14	8	-8	.000	.247	-.247
14	10	-8	.000	-.742	.742
*14	12	-8	.000	-1.052	1.052
15	1	-8	1.525	1.489	.036
15	3	-8	.676	.864	-.188
15	5	-8	.430	.592	-.161
15	7	-8	.568	.919	-.351
15	9	-8	1.269	1.276	-.006
15	11	-8	.000	1.043	-.1043
16	0	-8	1.815	1.850	-.034
16	2	-8	1.014	.952	.063
16	4	-8	.000	.413	-.413
16	6	-8	.000	-.235	.235
16	8	-8	1.476	1.321	.155
16	10	-8	1.333	1.425	-.092
17	1	-8	1.250	-1.145	-.104
17	3	-8	1.297	-1.307	.010
17	5	-8	.000	-.617	.617
17	7	-8	.000	-.210	.210
18	0	-8	.944	-.688	-.256

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18	4	-8	.000	.698	-.698
18	6	-8	.000	.498	-.498
0	0	9	1.297	-1.425	.128
0	2	9	.000	.095	-.095
0	4	9	2.810	2.392	.419
0	6	9	2.488	2.319	.169
1	1	9	.000	.483	-.483
1	1	-9	.000	.057	-.057
1	3	9	.000	.173	-.173
1	3	-9	.000	.522	-.522
1	5	9	.000	-.114	.114
1	5	-9	.771	.859	-.087
1	7	-9	.000	.399	-.399
1	9	-9	.000	-.224	.224
2	0	-9	2.197	2.028	.169
2	2	-9	.878	.905	-.027
2	4	-9	1.075	-1.125	.050
2	6	-9	1.310	-1.400	.089
2	8	-9	.000	.717	-.717
2	10	-9	1.595	1.573	.022
3	1	-9	.000	.366	-.366
3	3	-9	.000	-.423	.423
3	5	-9	.000	-.761	.761
3	7	-9	.000	.015	-.015
3	9	-9	.000	-.033	.033
3	11	-9	.000	.003	-.003
4	0	-9	.000	-.000	.000
4	2	-9	1.332	1.455	-.124
4	4	-9	2.805	2.818	-.013
4	6	-9	2.155	2.360	-.205
4	8	-9	.000	.414	-.414
4	10	-9	.000	.558	-.558
4	12	-9	1.085	1.052	.033
5	1	-9	.914	-.925	.011
5	3	-9	.000	-.525	.525
5	5	-9	.000	-.427	.427
5	7	-9	.000	-.179	.179
5	9	-9	.704	-.994	.290
5	11	-9	.000	-.706	.706
6	0	-9	.409	-.260	-.149
6	2	-9	1.022	-.903	-.119
6	4	-9	1.195	-1.150	-.045
6	6	-9	.000	-.290	.290
6	8	-9	.639	-.511	-.128
6	10	-9	1.265	-1.122	-.142
6	12	-9	.000	-.515	.515
7	1	-9	.000	-.619	.619
7	3	-9	.000	1.212	-.212
7	5	-9	.000	.544	-.544
7	7	-9	.000	-.897	.897
7	9	-9	.000	-.562	.562
7	11	-9	.000	1.122	-.122
7	13	-9	.000	-.077	.077
8	0	-9	.000	.204	-.204
8	2	-9	.566	.565	.001
8	4	-9	.971	-1.079	.107
8	6	-9	.000	.085	-.085
8	8	-9	.000	-.217	.217
8	10	-9	.000	.406	-.406
8	12	-9	.000	.114	-.114
9	1	-9	.000	.719	-.719

9	3	-9	.797	-.778	-.019
9	5	-9	.000	.030	-.030
9	7	-9	1.840	1.811	.030
9	9	-9	.000	-.070	.070
9	11	-9	.000	-.746	.746
9	13	-9	.000	-.700	.700
10	0	-9	3.062	-3.228	.166
10	2	-9	1.514	-1.521	.007
10	4	-9	.000	-.187	.187
10	6	-9	.640	-.682	.042
10	8	-9	1.230	-1.276	.046
10	10	-9	1.277	-1.449	.172
10	12	-9	1.740	-1.755	.014
11	1	-9	2.087	2.044	.044
11	3	-9	1.577	1.590	-.013
11	5	-9	.580	.501	.079
11	7	-9	.548	.794	-.245
11	9	-9	.443	.860	-.418
11	11	-9	2.260	2.327	-.067
12	0	-9	2.180	2.049	.132
12	2	-9	1.742	1.719	.023
12	4	-9	1.605	-1.589	-.016
12	6	-9	.000	-.273	.273
12	8	-9	.000	-.019	.019
12	10	-9	2.354	2.138	.216
12	12	-9	1.677	1.509	.168
13	1	-9	1.474	-1.397	-.077
13	3	-9	.904	.834	.071
13	5	-9	1.069	.828	.241
13	7	-9	.000	.184	-.184
13	9	-9	.000	-.694	.694
13	11	-9	.000	-.601	.601
14	0	-9	2.480	-2.645	.166
14	2	-9	.897	-.757	-.140
14	4	-9	1.591	1.667	-.076
14	6	-9	2.124	1.888	.236
14	8	-9	.000	-.659	.659
14	10	-9	2.282	-2.153	-.129
15	1	-9	.000	1.009	-.1.009
15	3	-9	.000	-.460	.460
15	5	-9	.000	-.893	.893
15	7	-9	.000	.319	-.319
15	9	-9	.000	.302	-.302
16	0	-9	1.396	1.360	.036
16	2	-9	1.532	1.376	.156
16	4	-9	.992	-1.170	.179
16	6	-9	.308	-.475	.167
16	8	-9	.000	.801	-.801
17	1	-9	2.662	-2.550	-.112
17	3	-9	.000	-.923	.923
17	5	-9	.000	-.262	.262
18	0	-9	1.758	-1.270	-.488
18	2	-9	.000	-.861	.861
2	0	-10	.000	.320	-.320
2	2	-10	.000	-.138	.138
2	4	-10	.000	.221	-.221
3	1	-10	.000	.035	-.035
3	3	-10	1.208	-.1.294	.086
3	5	-10	.000	-.598	.598
4	0	-10	2.513	1.667	.846
4	2	-10	.000	.577	-.577
4	4	-10	.000	.641	-.641

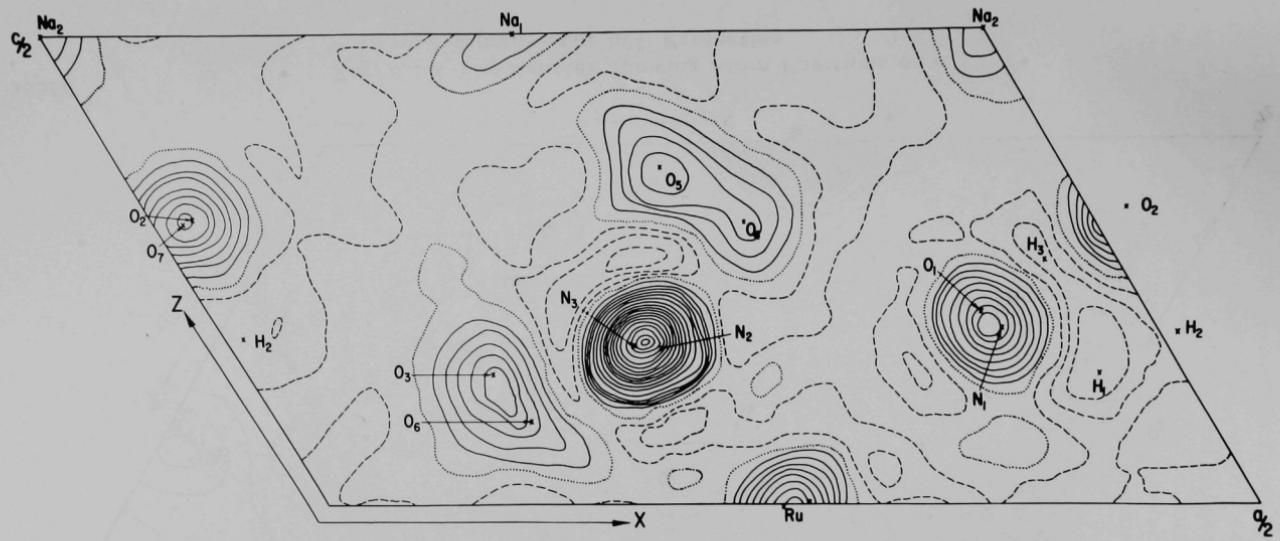
Isotopesmith-	4	6 -10	.000	-.692	.692
* 5	1	-10	.000	-.931	.931
* 5	3	-10	.000	.226	-.226
* 5	5	-10	.000	.275	-.275
* 5	7	-10	.000	-.992	.992
6	0	-10	1.770	-.1.773	.002
6	2	-10	2.214	-2.214	-.000
6	4	-10	.000	-.008	.008
6	6	-10	.000	.040	-.040
6	8	-10	1.273	-1.228	-.045
7	1	-10	1.503	1.423	.080
7	3	-10	.000	.230	-.230
7	5	-10	.000	-.234	.234
7	7	-10	.000	.065	-.065
7	9	-10	1.912	1.746	.165
8	0	-10	2.414	2.551	-.137
8	2	-10	.000	.296	-.296
8	4	-10	.000	-.592	.592
8	6	-10	1.581	-1.763	.182
8	8	-10	1.241	1.242	-.001
9	1	-10	.740	-.799	.059
9	3	-10	.000	.363	-.363
9	5	-10	2.189	2.276	-.086
9	7	-10	.000	.486	-.486
9	9	-10	.000	-1.013	1.013
10	0	-10	2.151	-2.280	.129
10	2	-10	1.067	-1.269	.202
10	4	-10	1.463	1.413	.050
10	6	-10	.714	.928	-.214
10	8	-10	.000	-.653	.653
11	1	-10	2.424	2.090	.335
11	3	-10	.000	-.217	.217
11	5	-10	1.029	-1.351	.322
11	7	-10	.000	-.098	.098
11	9	-10	2.668	2.527	.141
12	0	-10	3.926	4.114	-.188
12	2	-10	1.047	.996	.052
12	4	-10	.000	-.624	.624
12	6	-10	1.048	-1.093	.045
12	8	-10	2.010	1.925	.085
13	1	-10	2.546	-2.192	-.354
13	3	-10	.000	-.769	.769
13	5	-10	.000	.405	-.405
13	7	-10	.000	-.792	.792
14	0	-10	2.272	-2.489	.216
14	2	-10	.000	-.693	.693
14	4	-10	1.665	1.594	.071
14	6	-10	.000	.793	-.793
*15	1	-10	.000	.272	-.272
*15	3	-10	.000	-.748	.748
*15	5	-10	.000	-1.102	1.102
16	0	-10	1.662	1.492	.170
16	2	-10	.000	-.239	.239
16	4	-10	.000	-.908	.908
* 8	0	-11	.000	2.019	-.019
*10	0	-11	.000	-.978	.978
*12	0	-11	.000	.589	-.589

Although as indicated previously 2-dimensional Pattersons were used for a start on the structure, 3-dimensional Pattersons and 3-dimensional Fouriers gave a great deal more assistance in working out the details of the structure. For purposes of illustrating the relative positions of the atoms, we have included a 2-dimensional $h0\ell$ neutron Fourier, since in this projection the overlap is not too objectionable. This projection as shown in Figure 7 shows the nitrogens to be the heavy scatterers, although all atoms with a positive neutron scattering amplitude show up reasonably strong and the hydrogens with a negative scattering amplitude are also evident. After the determination of crystal structure was quite far along, X-ray zone data was gathered by use of a small spherically shaped crystal on a single-crystal orienter. MoK α radiation was used to obtain peak intensities of 126 ($h0\ell$) reflections, which were converted to F_{obs} values in the usual way, and the X-ray ($h0\ell$) Fourier map shown in Figure 8 was calculated. Although it is not claimed that these are the best possible X-ray intensity data obtainable, they do indeed show, as expected, the relatively low intensities scattered from all the light atoms in comparison with the heavy Ru atom.

Figure 9, which is a section of the $h0\ell$ 3-dimensional Fourier at $y = 0$, serves two purposes, namely, it illustrates the typical sharp, well-defined 3-dimensional Fourier peaks obtained at all levels, and also shows graphically the relative position of HO-Ru-NO groups. It will be recalled that their location, especially the Ru-NO bonding, was indicated as a reason for pursuing this investigation.

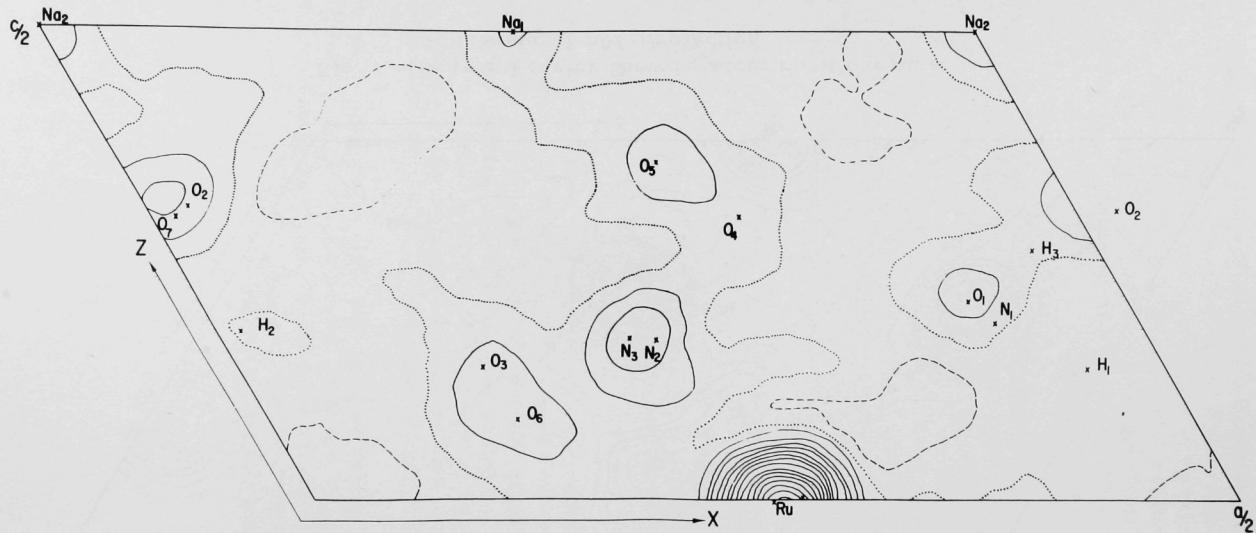
As indicated above, the refinement was carried out by successive F_0 and F_C syntheses; therefore, we have included a comparison in Table VI of the atom locations based on the two Fouriers together with the least-squares results. The location of the peaks and their heights was obtained by the use of a computer program.⁽¹⁶⁾ It can be noted that there was reasonably good agreement between the three results, with the H₂ and H₃ atoms of the water molecule showing the greatest difference.

We were concerned about the effect of having left out the 301 reflections; therefore, we ran a Fourier using the F_{calc} values with and without these reflections. The results showing coordinates and peak heights are summarized in Table VII. A slight difference can be noted in some coordinates, especially H₁ and H₂ atoms, but in general the agreement is quite good.



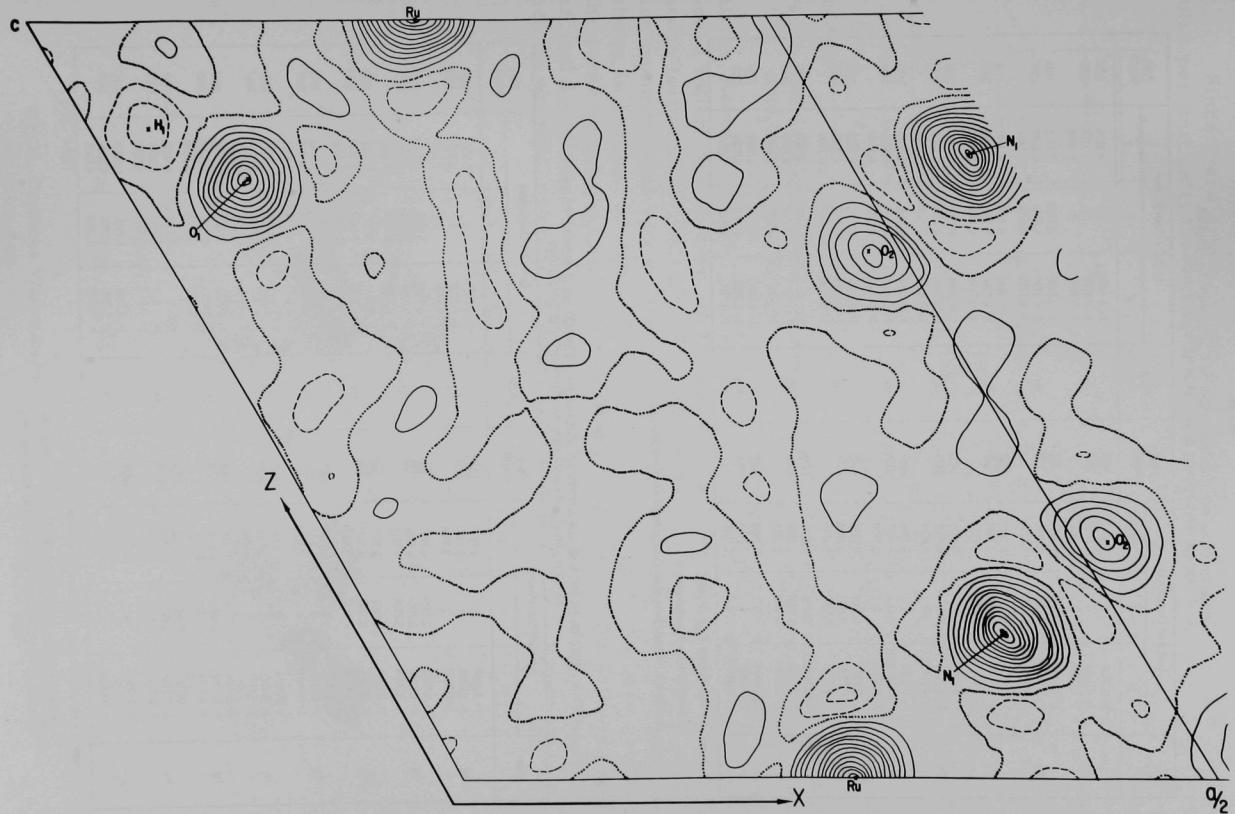
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Fig. 7. Neutron Fourier Showing Atom Positions on a
2-dimensional $h0l$ Projection



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Fig. 8. X-ray Fourier Showing Atom Positions on a
2-dimensional $h0\ell$ Projection



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Fig. 9. Section of $h0\ell$ 3-dimensional Neutron Fourier at $y = 0$ Showing the Relative Location of HO-Ru-NO Groups

Table VI

COMPARISON OF THE ATOM LOCATIONS BASED ON F_{calc} FOURIER, F_{obs} FOURIER,
AND THE LEAST-SQUARES RESULTS FROM THE BC REFLECTIONS

Atom	Unit Cell Coordinates			Peak Height	Atom	Unit Cell Coordinates			Peak Height
	x	y	z			x	y	z	
H_1	*1- 0.0407	0	0.8662	1054	O_2	*1- 0.5195	0	0.3116	2234
	2- 0.0403	0	0.8658	1048		2- 0.5199	0	0.3124	2208
	3- 0.0454	0	0.8607			3- 0.5201	0	0.3086	
H_2	1- 0.4847	0.2813	0.1739	756	O_3	1- 0.1295	0.1088	0.1452	1964
	2- 0.4828	0.2787	0.1730	702		2- 0.1295	0.1081	0.1467	1977
	3- 0.4871	0.2939	0.1806			3- 0.1288	0.1104	0.1402	
H_3	1- 0.4552	0.2211	0.2714	602	O_4	1- 0.3149	0.1460	0.3040	2138
	2- 0.4538	0.2225	0.2584	648		2- 0.3158	0.1463	0.3048	2061
	3- 0.4610	0.2189	0.2754			3- 0.3146	0.1472	0.3022	
Ru	1- 0.2608	0	0.0027	5636	O_5	1- 0.2098	0.1105	0.6373	2687
	2- 0.2608	0	0.0027	5575		2- 0.2100	0.1106	0.6370	2660
	3- 0.2619	0	0.0032			3- 0.2118	0.1116	0.6380	
N_1	1- 0.4212	0	0.1916	6058	O_6	1- 0.3644	0.1566	0.9122	1623
	2- 0.4210	0	0.1911	6018		2- 0.3622	0.1591	0.9121	1586
	3- 0.4205	0	0.1906			3- 0.3675	0.1559	0.9143	
N_2	1- 0.2305	0.0007	0.1720	6188	O_7	1- 0.0110	0.2321	0.3022	2390
	2- 0.2298	0.0111	0.1704	6055		2- 0.0118	0.2319	0.3033	2466
	3- 0.2313	0.0002	0.1716			3- 0.0106	0.2307	0.2999	
N_3	1- 0.2834	0.1024	0.8277	6522	Na_1	1- 0	0.1106	0.5000	1930
	2- 0.2835	0.1024	0.8278	6390		2- 0	0.1109	0.5000	1948
	3- 0.2839	0.1024	0.8284			3- 0	0.1089	0.5000	
O_1	1- 0.0859	0	0.7918	3945	Na_2	1- 0.2500	0.2500	0.5000	1525
	2- 0.0857	0	0.7918	3866		2- 0.2500	0.2500	0.5000	1472
	3- 0.0877	0	0.7907			3- 0.2500	0.2500	0.5000	

* Note: 1 - Results from F_{calc} Fourier.

2 - Results from F_{obs} Fourier.

3 - Results from last least-squares cycle based on BC reflections.

Table VII

EFFECT OF THE MISSING REFLECTIONS AS INDICATED BY A COMPARISON OF ATOM LOCATIONS
BASED ON AN F_{calc} FOURIER WITH AND WITHOUT THESE REFLECTIONS

Atom	Unit Cell Coordinates			Peak Height	Atom	Unit Cell Coordinates			Peak Height
	x	y	z			x	y	z	
H_1	*1- 0.0554	0	0.8575	1742	O_2	*1- 0.5273	0	0.3088	2670
	2- 0.0406	0	0.8634	1127		2- 0.5207	0	0.3117	2262
	3- 0.0449	0	0.8606			3- 0.5210	0	0.3094	
H_2	1- 0.5083	0.2909	0.1841	685	O_3	1- 0.1303	0.1098	0.1430	2467
	2- 0.4884	0.2781	0.1840	858		2- 0.1298	0.1084	0.1465	2134
	3- 0.5086	0.2920	0.1811			3- 0.1288	0.1094	0.1420	
H_3	1- 0.4653	0.2201	0.2727	943	O_4	1- 0.3132	0.1472	0.3002	2769
	2- 0.4668	0.2200	0.2679	690		2- 0.3133	0.1465	0.3012	2243
	3- 0.4631	0.2190	0.2675			3- 0.3146	0.1474	0.3020	
Ru	1- 0.2625	0	0.0039	6829	O_5	1- 0.2131	0.1115	0.6406	3092
	2- 0.2618	0	0.0034	5947		2- 0.2104	0.1113	0.6393	2737
	3- 0.2623	0	0.0037			3- 0.2123	0.1118	0.6391	
N_1	1- 0.4134	0	0.2096	4622	O_6	1- 0.3663	0.1552	0.9129	2029
	2- 0.4270	0	0.2011	6100		2- 0.3647	0.1558	0.9109	1667
	3- 0.4197	0	0.1892			3- 0.3685	0.1552	0.9149	
N_2	1- 0.2306	0.1005	0.1716	6866	O_7	1- 0.0116	0.2302	0.3010	2787
	2- 0.2302	0.1005	0.1718	6254		2- 0.0110	0.2309	0.3023	2455
	3- 0.2311	0.1002	0.1714			3- 0.0120	0.2304	0.3016	
N_3	1- 0.2165	0.3973	0.1731	7159	Na_1	1- 0	0.1091	0.5000	2103
	2- 0.2168	0.3972	0.1729	6563		2- 0	0.1091	0.5000	1923
	3- 0.2165	0.3977	0.1723			3- 0	0.1097	0.5000	
O_1	1- 0.0866	0	0.7904	4621	Na_2	1- 0.2500	0.2500	0.5000	1611
	2- 0.0857	0	0.7910	4088		2- 0.2500	0.2500	0.5000	1469
	3- 0.0875	0	0.7904			3- 0.2500	0.2500	0.5000	

* Note: 1 - Results from F_{calc} Fourier based on all reflections.

2 - Results from F_{calc} Fourier after removing missing reflections.

3 - Results from last least-squares cycle based on ABC reflections.

DISCUSSION OF THE STRUCTURE

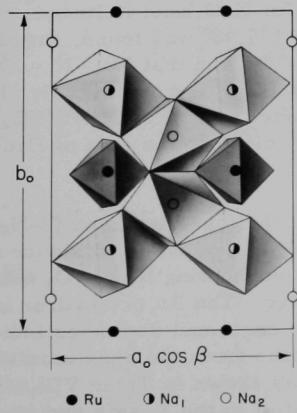
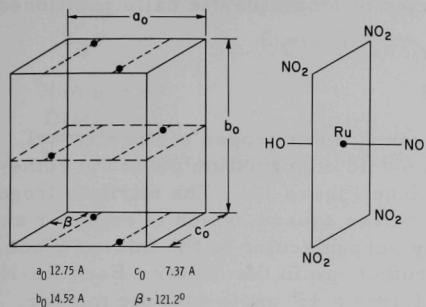
Since there are eight general positions in C_2/m and only four molecules per unit cell, the atoms are distributed over both special and general positions.

The ruthenium, nitrosyl, and hydroxyl are in special positions on the mirror plane; the sodiums occupy two sets of special positions, one on a center of symmetry and one on a two-fold axis; and the nitrito groups and waters are in general positions. The relative locations of the Ru atoms within the unit cell are shown in Figure 10, where it is evident that the Ru atoms are very close to $1/4, 0, 0$ and equivalent positions.

106-7082

Fig. 10. Lattice Constants and Schematic Structure of $\text{Na}_2[\text{Ru}(\text{NO}_2)_4\text{NO}\cdot\text{OH}] \cdot 2\text{H}_2\text{O}$

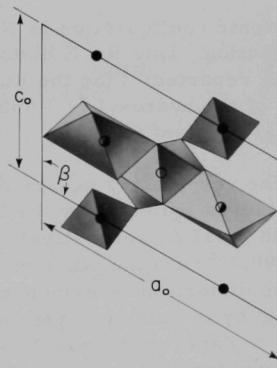
atoms, namely, the Ru, Na_1 , and Na_2 forming three different kinds of octahedra which include most of the atoms within the structure. These octahedra form an interlocking chain throughout the structure, in which there are common atoms or common edges shared between the octahedra, as shown in Figures 11 and 12. Each of the three octahedra have relatively the same orientation within the cell. Four atoms in each are arranged around a central atom in a near coplanar square which is perpendicular or nearly perpendicular to the mirror plane or parallel to the b axis. The



106-7627

Fig. 11. Octahedra Viewed Down the c Axis

The structure can be envisioned as consisting mainly of 6-fold coordination about three central



106-7628

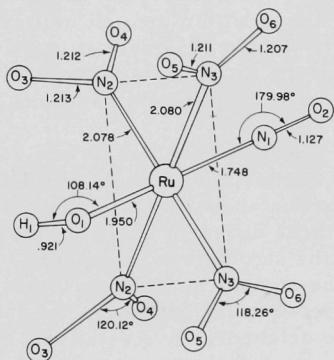
Fig. 12. Octahedra Viewed Down the b Axis

other two atoms involved in the 6-fold coordination group lie along a line perpendicular or nearly perpendicular to this square plane and nearly parallel to the mirror plane, thus forming the octahedra. In order to better envisage this structure a model consisting of two complete unit cells (100 atoms per unit cell) was constructed of small plastic balls positioned on rods parallel to the "b" axis.

A. Configuration about the Ruthenium

Four nitrogens of the nitrito groups, the nitrogen of the nitrosyl, and the oxygen of the hydroxyl form a 6-fold coordination about the ruthenium (see Figure 13).

The nitrito nitrogens form a near square, which is coplanar and nearly perpendicular to the mirror plane with ruthenium in the center. Each Ru-N bond forms a 45° angle with the mirror. The NO and OH groups lie in the mirror, trans with respect to the ruthenium, and the N₁ of the nitrosyl and the O₁ of the hydroxyl are at the apices of the octahedron.



106-7630

Fig. 13. Configuration about the Ruthenium Atom

The electronic configuration is Ru = N = O: and that Ru - N = O: makes no contribution. This Ru-N distance of 1.748 Å is considerably shorter than the 1.85 Å reported⁽⁵⁾ for the Ru-N distance in K₂[RuNO(OH)(NO₂)₄]. The Ru to O of the hydroxyl is 1.950 Å, very close to the sum of Pauling's octahedral covalent radii.

The very nearly square nature of the four nitrogens (2-N₂ and 2-N₃) about the Ru is indicated by the N₂-N₂, N₃-N₃ and N₂-N₃ distances of 2.909, 2.972, and 2.937 Å, respectively. A link connecting N₁ and O₁ makes an angle of 90.33° with the plane of the square. The Ru octahedron contains very little distortion as evidenced by the angle and distances indicated above, and by the almost equal edge lengths from the apex atoms N₁ and O₁ to the coplanar nitrogens N₂ and N₃, as shown in Table VIII A3. The plane shown dashed in Figure 13 is parallel to the y axis and is rotated 11.2° counterclockwise from the z axis. The N-O distance in the nitrosyl is 1.127 Å, which is in good agreement with 1.1 Å reported by Bokii, Ang-nu, and Khodashova⁽⁵⁾ for K₂[RuNO(OH)(NO₂)₄], but the angle of 179.98° is in

Table VIII

SOME INTER- AND INTRAMOLECULAR BOND DISTANCES⁽¹⁾ AND ANGLESA. Configuration about the Ruthenium

<u>Number of Distances</u>	<u>Atom 1</u>	<u>Atom 2</u>	<u>Distance, Å</u>
1. Ru to closest neighbors (6-fold coordination)			
1	Ru	N ₁ (NO)	1.748 (4)
2	Ru	N ₂ (NO ₂) ₂	2.078 (3)
2	Ru	N ₃ (NO ₂) ₃	2.080 (3)
1	Ru	O ₁ (OH)	1.950 (5)
2. Nitrogen "square" about Ru			
1	N ₃ (NO ₂) ₃	N ₃ (NO ₂) ₃	2.972 (4)
2	N ₂ (NO ₂) ₂	N ₃ (NO ₂) ₃	2.937 (3)
1	N ₂ (NO ₂) ₂	N ₂ (NO ₂) ₂	2.909 (4)
3. Ru octahedron edges			
2	N ₁ (NO)	N ₂ (NO ₂) ₂	2.754 (3)
2	N ₁ (NO)	N ₃ (NO ₂) ₃	2.744 (3)
2	O ₁ (OH)	N ₂ (NO ₂) ₂	2.831 (4)
2	O ₁ (OH)	N ₃ (NO ₂) ₃	2.798 (4)
4. Vicinity of the Ru octahedron			
1	N ₁ (NO)	O ₂ (NO)	1.127 (7)
2	N ₂ (NO ₂) ₂	O ₃ (NO ₂) ₂	1.213 (5)
2	N ₂ (NO ₂) ₂	O ₄ (NO ₂) ₂	1.212 (5)
2	N ₃ (NO ₂) ₃	O ₅ (NO ₂) ₃	1.211 (4)
2	N ₃ (NO ₂) ₃	O ₆ (NO ₂) ₃	1.207 (5)
1	H ₁ (OH) ₃	O ₁ (OH)	0.921 (9)
			0.974 (11)*
			1.038 (10)**
5. Angles - Ru octahedron			
<u>Atom 1</u>	<u>Atom 2</u>	<u>Atom 3</u>	<u>Angle, deg</u>
Ru	N ₁ (NO)	O ₂ (NO)	179.98 (55)
Ru	O ₁ (OH)	H ₁ (OH)	108.15 (67)
N ₁ (NO)	Ru	O ₁ (OH)	178.68 (26)
O ₃ (NO ₂)	N ₂ (NO ₂)	O ₄ (NO ₂)	120.12 (37)
O ₅ (NO ₂)	N ₃ (NO ₂)	O ₆ (NO ₂)	118.26 (37)
N ₂ (NO ₂)	Ru	N ₂ (NO ₂)	88.88 (17)

(1) Standard errors ($\times 10^3$) appear in parentheses.

Table VIII (Contd.)

<u>Atom 1</u>	<u>Atom 2</u>	<u>Atom 3</u>	<u>Angle, deg</u>
$\text{N}_2(\text{NO}_2)$	Ru	$\text{N}_3(\text{NO}_2)$	89.88 (8)
$\text{N}_3(\text{NO}_3)$	Ru	$\text{N}_3(\text{NO}_2)$	91.36 (11)
$\text{N}_1(\text{NO})$	Ru	$\text{N}_2(\text{NO}_2)$	91.75 (15)
$\text{O}_1(\text{OH})$	Ru	$\text{N}_2(\text{NO}_2)$	89.24 (15)

B. Configuration about the Sodium-1

<u>Number of Distances</u>	<u>Atom 1</u>	<u>Atom 2</u>	<u>Distance, Å</u>
1. Na_1 to closest neighbors (6-fold coordination)			
2	Na_1	$\text{O}_4(\text{NO}_2)_2$	2.505 (4)
2	Na_1	$\text{O}_5(\text{NO}_2)_3$	2.413 (4)
2	Na_1	$\text{O}_7(\text{H}_2\text{O})$	2.613 (6)
2. Oxygen "square" about Na_1			
2	$\text{O}_4(\text{NO}_2)_2$	$\text{O}_5(\text{NO}_2)_3$	3.392 (7)
2	$\text{O}_4(\text{NO}_2)_2$	$\text{O}_5(\text{NO}_2)_3$	3.562 (8)
3. Na_1 octahedron edges			
2	$\text{O}_7(\text{H}_2\text{O})$	$\text{O}_4(\text{NO}_2)_2$	3.140 (7)
2	$\text{O}_7(\text{H}_2\text{O})$	$\text{O}_4(\text{NO}_2)_2$	4.043 (7)
2	$\text{O}_7(\text{H}_2\text{O})$	$\text{O}_5(\text{NO}_2)_3$	3.014 (6)
2	$\text{O}_7(\text{H}_2\text{O})$	$\text{O}_5(\text{NO}_2)_3$	3.552 (8)
4. Vicinity of the Na_1 octahedron			
2	Na_1	$\text{O}_3(\text{NO}_2)_2$	3.049 (5)
2	Na_1	$\text{O}_6(\text{NO}_2)_3$	2.957 (6)

C. Configuration about the Sodium-2

1.	Na_2 to closest neighbors (6-fold coordination)		
2	Na_2	$\text{O}_1(\text{OH})$	2.430 (7)
2	Na_2	$\text{O}_7(\text{H}_2\text{O})$	2.335 (8)
2	Na_2	$\text{O}_5(\text{NO}_2)_3$	2.345 (5)
2. Oxygen "square" about Na_2			
1	$\text{O}_1(\text{OH})$	$\text{O}_1(\text{OH})$	3.669 (8)
2	$\text{O}_1(\text{OH})$	$\text{O}_7(\text{H}_2\text{O})$	3.518 (6)
1	$\text{O}_7(\text{H}_2\text{O})$	$\text{O}_7(\text{H}_2\text{O})$	3.088 (9)

Table VIII (Contd.)

3. Na_2 octahedron edges

<u>Atom 1</u>	<u>Atom 2</u>	<u>Distance, Å</u>
$\text{O}_5(\text{NO}_2)_3$	$\text{O}_7(\text{H}_2\text{O})$	3.014 (6)
$\text{O}_5(\text{NO}_2)_3$	$\text{O}_7(\text{H}_2\text{O})$	3.552 (8)
$\text{O}_5(\text{NO}_2)_3$	$\text{O}_1(\text{OH})$	2.875 (6)
$\text{O}_5(\text{NO}_2)_3$	$\text{O}_1(\text{OH})$	3.839 (6)

D. Bond Distances and Angles between O-O
(Possible Hydrogen Bonding)

<u>Atom 1</u>	<u>Atom 2</u>	<u>Atom 3</u>	<u>1-3 Distance</u>	<u>1-2-3 Angle</u>
$\text{O}_7(\text{H}_2\text{O})$		$\text{O}_1(\text{OH})$	3.518 (6)	
$\text{O}_7(\text{H}_2\text{O})$		$\text{O}_2(\text{NO})$	3.916 (5)	
$\text{O}_7(\text{H}_2\text{O})$	$\text{H}_2(\text{H}_3)$	$\text{O}_3(\text{NO}_2)$	2.919 (7)	139° (29°)
$\text{O}_7(\text{H}_2\text{O})$	$\text{H}_2(\text{H}_3)$	$\text{O}_3(\text{NO}_2)$	3.308 (9)	131° (63°)
$\text{O}_7(\text{H}_2\text{O})$	$\text{H}_2(\text{H}_3)$	$\text{O}_4(\text{NO}_2)$	3.079 (7)	43° (145°)
$\text{O}_7(\text{H}_2\text{O})$	$\text{H}_2(\text{H}_3)$	$\text{O}_4(\text{NO}_2)$	3.140 (7)	46° (81°)
$\text{O}_7(\text{H}_2\text{O})$	$\text{H}_2(\text{H}_3)$	$\text{O}_5(\text{NO}_2)$	3.014 (6)	59° (63°)
$\text{O}_7(\text{H}_2\text{O})$	$\text{H}_2(\text{H}_3)$	$\text{O}_5(\text{NO}_2)$	3.552 (8)	78° (23°)
$\text{O}_7(\text{H}_2\text{O})$	$\text{H}_2(\text{H}_3)$	$\text{O}_6(\text{NO}_2)$	2.972 (8)	103° (119°)
$\text{O}_7(\text{H}_2\text{O})$	$\text{H}_2(\text{H}_3)$	$\text{O}_6(\text{NO}_2)$	3.187 (7)	96° (80°)
$\text{O}_7(\text{H}_2\text{O})$		$\text{O}_7(\text{H}_2\text{O})$	3.088 (9)	
$\text{O}_3(\text{NO}_2)$	H_1	$\text{O}_1(\text{OH})$	2.842 (6)	135°
$\text{O}_3(\text{NO}_2)$	H_1	$\text{O}_1(\text{OH})$	3.433 (7)	110°
$\text{O}_5(\text{NO}_2)$	H_1	$\text{O}_1(\text{OH})$	2.875 (6)	
$\text{O}_3(\text{NO}_2)$		$\text{O}_3(\text{NO}_2)$	2.838 (10)	
$\text{O}_3(\text{NO}_2)$		$\text{O}_3(\text{NO}_2)$	3.175 (14)	
		$\text{O}_2(\text{NO})$		

E. H_2O Distances and Angle

<u>Atom 1</u>	<u>Atom 2</u>	<u>Atom 3</u>	<u>Distance Angle</u>
H_2		$\text{O}_7(\text{H}_2\text{O})$	0.929 (16) 1.061 (19)* 1.185 (18)**
H_3		$\text{O}_7(\text{H}_2\text{O})$	0.911 (14) 1.000 (15)* 1.130 (14)**
$\text{H}_2(\text{H}_2\text{O})$		$\text{H}_3(\text{H}_2\text{O})$	1.500 (26)
H_2	O_7	H_3	$109.3 \pm 1.9^\circ$

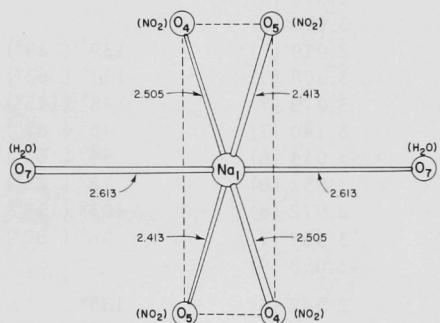
*Assumed that H rides on O.

**Assumed that the H and O move independently.

disagreement with their reported value of $\sim 170^\circ$. The Ru-O₁-H₁ angle is 108.15° and the O-H distance is 0.921 \AA as calculated with parameters averaged over temperature motion. A 0.974 \AA distance is found if the hydrogen is assumed to ride on the oxygen and a 1.038 \AA distance if the two atoms are assumed to move independently. The O₁-Ru-N₁ angle is 178.68° . The N-O distances and angles of the nitrito groups are in good agreement with accepted values, with the following distances obtained for the four unique N-O bonds: 1.213, 1.212, 1.211, and 1.207 \AA . The two O-N-O angles are 120.12° and 118.26° .

B. Configuration about the Sodium-1

The 6-fold coordination about the Na₁ consists of 6 oxygen atoms, four from NO₂ groups and two from water molecules, as shown in Figure 14.



106-7629-A

Fig. 14. Configuration about the Sodium-1 Atom

two different NO₂ groups; and 2 at 2.613 \AA from the waters. The average Na-O distance of the above, namely, 2.510 \AA , is within the 2.25 - 2.78 \AA range reported⁽¹⁷⁾ for 6-fold coordination from 16 previous determinations and only slightly higher than the 2.44 \AA average reported for these same compounds.

The two sets of O-O distances along the edges of the distorted square, namely, 3.392 and 3.562 \AA , indicate the extent of the distortion to a parallelogram. A line through O₇-Na₁-O₇ forms an angle of approximately 68° to the parallelogram and is tilted approximately 6.3° from the ac face. The distortion of the octahedron is evident by the different edge lengths from the apex atoms, O₇, to the coplanar oxygen atoms, O₄ and O₅, as shown in Table VIIIB3.

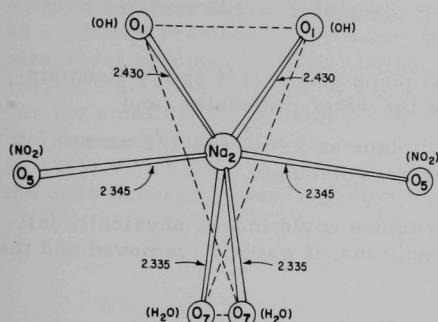
The four oxygens of the NO₂ groups are coplanar and are arranged in a parallelogram with the Na₁ at the center, since the Na₁ is at a center of symmetry. This parallelogram, shown dashed, is tilted approximately 1.1° from the y axis and is rotated approximately 19.7° counter-clockwise from the z axis. Oxygens from each of two water molecules are at the apices of the octahedron, which has approximately the same relative orientation as the Ru octahedron described above.

The distances from the central Na₁ atom to its nearest oxygen neighbors are as follows: 2 at 2.413 \AA and 2 at 2.505 \AA from the

It is also interesting to note that there are four other oxygen atoms fairly close to the Na_1 . These are two $\text{O}_3(\text{NO}_2)$ at 3.049 \AA and two $\text{O}_6(\text{NO}_2)$ at 2.957 \AA which are not a part of the three basic octahedra - Ru, Na_1 , or Na_2 . Further comments will be made about these later.

C. Configuration about the Sodium-2

The 6-fold coordination about the Na_2 consists of six oxygen atoms: two from hydroxyls, two from nitritos, and two from waters, as shown in



38890

Fig. 15. Configuration about the Sodium-2 Atom

Figure 15. Two oxygens from hydroxyls and two from waters are arranged in a greatly distorted square about a nearly central Na_2 atom. Because the Na_2 is on a two-fold axis it is not required to be at the center of this square. Two O_5 from nitritos are at the apices of the octahedron.

The distances from the central Na_2 atom to its nearest oxygen neighbors are as follows: two $\text{O}_1(\text{OH})$ at 2.430 \AA ; two $\text{O}_7(\text{H}_2\text{O})$ at 2.335 \AA ; two $\text{O}_5(\text{NO}_2)$ at 2.345 \AA . The average distance, 2.370 \AA , is somewhat lower than the average 2.510 \AA found for the Na_1 octahedron

above and also is even lower than the average 2.44 \AA reported⁽¹⁷⁾ previously for the 16 compounds. However, the average of all 12 Na-O distances is, coincidentally, 2.44 \AA .

In the case of the Na_2 octahedron the two O_1 's (OH) and two O_7 's (H_2O) form a greatly distorted square as indicated by the sides of 3.669 \AA , 2 of 3.518 \AA , and 3.088 \AA . The plane of this square is also greatly twisted as indicated by the fact that the O_1 and O_7 atoms lie approximately 0.46 \AA and 0.51 \AA , respectively, from the least-squares plane containing the O_1 , O_7 , and Na_2 atoms. The normal of this plane makes an angle of 7.5° with the line joining the O_5 - O_5 and is parallel to the ac plane. The least-squares plane is rotated 13.5° counterclockwise from the z axis. The skewed nature of this Na_2 octahedron is also evident from the variation of the edge lengths, ranging from 2.875 to 3.552 \AA as shown in Table VIIIC3.

D. General Features of the Structure

It is interesting to examine the structure of this compound on the basis of the octahedron-octahedron linkage as shown in Figures 11 and 12. The Ru octahedra are linked to the Na_2 octahedra through a common O_1 atom; the Na_1 octahedra are linked to Na_2 octahedra by a common edge

formed by O₅-O₇ atoms; the Na₂ octahedrons are linked to other Na₂ octahedrons by a common edge of O₁-O₁. This arrangement leaves all octahedra interconnected. The only atoms not included in these octahedra are: H₁(OH), O₂(NO), H₂ and H₃(H₂O), and O₃ and O₆(NO₂).

Each Ru octahedron may also be viewed as being surrounded and separated from other Ru octahedra by sheets of Na atoms and H₂O molecules as follows:

- (1) a sheet parallel to the (001) plane at z = 1/2 contains only Na₁ and Na₂ atoms;
- (2) sheets parallel to the (010) plane at y = 1/4 and 3/4 contain Na₁ atoms and O₇ atoms of the water molecules, and
- (3) sheets parallel to the (100) plane at x = 0 and 1/2 contain Na₂ and O₇ atoms of the water molecules.

Thus, it seems reasonable that the structure could indeed physically fall apart, as it did under low humidity conditions, if water is removed and the Na-O bonds are broken.

It is also of interest to determine the possible role of hydrogen bonding in the structure. In Table VIIID the various O-O distances are given that might be involved in hydrogen bonding. All of the O₇(H₂O)-O distances appear to be rather large, although several fall within the range from 2.49 to 3.15 Å reported⁽¹⁸⁾ for 16 different inorganic salts containing water. The shortest O₇(H₂O)-O distances are observed with the O₃ and O₆, which have distances of 2.919 and 2.972 Å, respectively. These are the two oxygens which, as described before, are not involved with the 6-fold coordination about Na₁ or Na₂, and hence might be involved in a weak hydrogen bond. A hydrogen bond might be involved between O₇-H₂-O₃, which has an angle of 139° and a distance of 2.919 Å, and O₇-H₃-O₆, which has an angle of 119° and a distance of 2.972 Å. These angles, however, are rather small in terms of an average of 167° found for 15 compounds as recently reported.⁽¹⁹⁾ Perhaps even more probable is an O₃-H₁-O₁ hydrogen bond, which involves a slightly closer distance, 2.842 Å, and an angle of 135°. The relative different environment between the O₃ and O₆ as shown above may indeed make the NO₂ groups about the Ru somewhat different: 2-NO₂ groups involving O₃ and 2-NO₂ involving O₆.

The various distances observed in the water molecule are summarized in Table VIIIE. Distances of 0.929 and 0.911 Å were observed for O-H bonds of the two hydrogens calculated with parameters averaged over temperature motion. These distances increased to 1.061 and 1.000 Å if it was assumed that the H rides on the O and somewhat greater distances if the H and O move independently. The H-O-H angle is 109.3°. Both

distances and angle agree favorably with other recent results⁽²⁰⁾ in which a value of approximately 1.0 Å for the O-H distance was observed and an angle of approximately 110°.

Calculations have also been made for the RMS radial thermal displacement and the RMS component along each principal axis. The results are shown in Table IX. The hydrogens, as might be expected, have large radial displacements, that of the water hydrogens being greater than that of the hydroxyl hydrogens. The O₃'s and O₆'s appear to have the largest displacements among the oxygens, which may be attributed to the fact that, as explained previously, these two oxygens seem to participate less in the structural bonding. The Na₁, which is located in the octahedron having the longest Na-O bonds, also has a large displacement. The heavy atom Ru has the smallest displacement and is essentially isotropic. The RMS radial thermal displacements are in agreement with the peak heights, listed in Table VI, of the F_{obs} Fourier map. Thus, among atoms of a given kind, the ones having the smallest displacements have the largest peak heights.

Table IX

RMS RADIAL THERMAL DISPLACEMENT AND THE RMS
COMPONENT ALONG EACH PRINCIPAL AXIS

Atom	RMS Radial, Å	RMS Component along the Three Principal Axes, Å		
H ₁ (OH)	0.425 (11)	0.150 (11)	0.203 (10)	0.342 (15)
H ₂ (H ₂ O)	0.647 (17)	0.216 (14)	0.393 (21)	0.467 (24)
H ₃ (H ₂ O)	0.575 (13)	0.195 (12)	0.361 (16)	0.403 (17)
Ru	0.255 (3)	0.143 (4)	0.149 (4)	0.149 (5)
N ₁ (NO)	0.305 (3)	0.154 (4)	0.180 (3)	0.191 (4)
N ₂ (NO ₂)	0.312 (2)	0.145 (3)	0.186 (3)	0.204 (3)
N ₃ (NO ₂)	0.301 (2)	0.146 (3)	0.184 (2)	0.187 (3)
O ₁ (OH)	0.289 (4)	0.153 (6)	0.162 (6)	0.185 (6)
O ₂ (NO)	0.416 (6)	0.155 (7)	0.270 (8)	0.276 (8)
O ₃ (NO ₂)	0.439 (5)	0.158 (6)	0.244 (5)	0.329 (7)
O ₄ (NO ₂)	0.407 (4)	0.161 (5)	0.230 (5)	0.294 (6)
O ₅ (NO ₂)	0.389 (4)	0.151 (5)	0.212 (5)	0.290 (6)
O ₆ (NO ₂)	0.517 (8)	0.156 (6)	0.214 (6)	0.443 (10)
O ₇ (H ₂ O)	0.400 (4)	0.180 (5)	0.214 (5)	0.285 (6)
Na ₁	0.434 (12)	0.162 (12)	0.179 (11)	0.360 (15)
Na ₂	0.358 (8)	0.167 (10)	0.176 (10)	0.264 (11)
Av.	0.404	0.162	0.222	0.291

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